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TRANSMISSION OF DOPPLER BROADENED RESONANCE RADIATION THROUGH ABSORBING MEDIA WITH COMBINED DOPPLER AND PRESSURE BROADENING (NITRIC OXIDE γ-BANDS AS AN EXAMPLE)

ENGINE TEST FACILITY
ARNOLD ENGINEERING DEVELOPMENT CENTER
AIR FORCE SYSTEMS COMMAND
ARNOLD AIR FORCE STATION, TENNESSEE 37389

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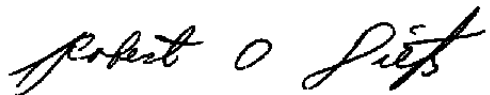| REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
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The combined Doppler and pressure broadening parameter has been determined for the 0,0 γ-band of nitric oxide (NO) by comparing measured spectral transmission data with the computed transmission using a radiative transfer model. The parameter (a', the ratio of collisional plus natural half-width to the Doppler half-width) was found to obey the relationship $a' = Cp/T$, where p is the pressure in atmospheres, T is the temperature in K, and C is a constant. The

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20. ABSTRACT (Continued)

value of C was found to be 1270 $\pm$ 200 K/atm. This value of C
leads to a value for the optical diameter of NO for broadening of
3.5 $\pm$ 0.3 Å. The determination of the broadening parameter
permits the accurate calculation of the transmission of NO γ-band
radiation through the high temperature, ambient pressure media
corresponding to jet engine exhausts, in turn making possible the
relating of transmission measurements to the concentration of NO.
The application of the measurement and calculation procedure to
the measurement problem is discussed.

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PREFACE

The research reported herein was conducted by the Arnold Engineering Development Center (AEDC), Air Force Systems Command (AFSC), under Program Element 65807F. The results were obtained by ARO, Inc. (a subsidiary of Sverdrup & Parcel and Associates, Inc.), contract operator of AEDC, AFSC, Arnold Air Force Station, Tennessee. The work was accomplished in the Engine Test Facility (ETF), under ARO Project Numbers R32P-54 and R32P-55A. The authors of this report were M. G. Davis, W. K. McGregor, J. D. Few, and H. N. Glassman, ARO, Inc. The manuscript (ARO Control No. ARO-ETF-TR-75-115) was submitted for publication on June 30, 1975.

Dr. M. G. Davis is an Associate Professor of Physics at the University of Tennessee at Nashville and consultant to ARO, Inc.

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1.0 INTRODUCTION

The radiative transfer of Doppler broadened spectral lines, contained within electronic-vibrational-rotational bands, through Doppler broadened absorbing media has been treated in a previous report (Ref. 1). In the work reported herein, the radiative transfer of Doppler broadened source bands through media with Doppler and collision broadened lines is treated. In Ref. 1, the nitric oxide (NO) molecule was used to demonstrate the technique and to compare experimental data from low-pressure, Doppler broadened absorbing media with the calculated band profiles. In the work reported herein, NO will be used again but at pressures such that collisional broadening by a foreign gas (N_2) is present. Knowledge of the collisional broadening parameter for NO was found to be uncertain (Ref. 2) so that a major part of the present work was the determination of the broadening parameter to a higher degree of accuracy over a large range of pressure and temperature conditions.

The application of this work is found in the use of spectral line transmission through high temperature media to determine species concentration and temperature in situ. Previously, measurements using this spectral line resonance absorption technique (Refs. 3 and 4) have been made using empirical procedures to account for the finite width of the source lines. The work reported in Ref. 1 permitted the measured transmission to be related to species concentration and temperature in a rigorous fashion when pressure (e. g., collisional) broadening could be neglected. The development in the present report will permit measurements to be related to species concentration and temperature over pressure ranges where the pressure broadening is comparable to, or dominates, the Doppler broadening.

The broadening parameter (a') as used in most treatments of spectral line broadening (Refs. 5 and 6, for example) is proportional to the ratio of the sum of the natural half-width and the collisional half-width of the line to the Doppler half-width. The natural half-width can be neglected for electronic resonance transitions. Theoretical estimating procedures are generally inadequate to predict the collisional broadening and measurements cannot separate the Doppler from the collisional contributions so that the parameter (a') must be experimentally determined. Direct measurement of the broadening half-width to determine a' requires high resolution

spectral instruments. In the treatment used in the present study, a theoretical calculation procedure is used to predict transmission from experimental·measurements, and thus by iteration of the calculations using a′ as a parameter, the value of a′ is indirectly determined by matching calculated and measured transmission. The required experimental data were obtained by measurement of the transmission of Doppler broadened lines in the (0, 0) γ-band of NO from a gas discharge lamp through a temperature-controlled (60 to 1, 000°F) absorption cell containing known mixtures of NO and N_2 at pressures varying from about 0. 1 to 2 atm.

The results of the theoretical development and the empirically determined value of a′ are applicable directly to calculations of the transmission of the (0, 0) γ-band of NO emitted by a resonance radiation source through absorbing media of various NO concentrations, pressures, and temperatures. The temperatures and pressures accessible in the calibration laboratory is limited, so that direct calibration for all possible conditions is not possible. However, the determination of a′ and the use of the theoretical relationships between the transmissivity and NO concentration permits extension to environments expected at the exhaust exit of combustion engines and other devices in which measurements of NO concentration might be desired.

2.0 THEORETICAL DEVELOPMENT

2.1 DEVELOPMENT OF TRANSMISSION FORMULAS FOR CASES INVOLVING ABSORPTION LINES BROADENED BY FOREIGN GASES

For a single, isolated j^{th} spectral line, the transmission $(\overline{T}_j)$ of a source line having some frequency distribution $(I^o_{\nu_j})$ through uniform absorbing medium of length ℓ is given by (Ref. 5):

$$\overline{T}_j = \int_o^\infty I^o_{\nu_j} \exp\left(-k_{\nu_j}\ell\right) d\nu \tag{1}$$

where ν is the frequency and k_{ν_j} is the absorption coefficient which has a frequency distribution independent of I_{ν_j}. If the radiation source is maintained at low pressure, the frequency distribution for I_{ν_j} can be attributed to the Doppler effect, and is given by

$$I^o_{\nu_j} = I^o_{\nu_j^c} \exp \left\{ -\left[\frac{2(\nu - \nu^o_j)}{(\Delta_s\nu_j)_D} \sqrt{\ln 2} \right]^2 \right\} \tag{2}$$

where $I^o_{\nu_j^c}$ is the intensity of the source line at center frequency (ν^o_j) and $(\Delta_s\nu_j)_D$ is the Doppler width at half the intensity (half-width) of the emitted spectral line. The Doppler half-width of the source line is given by

$$(\Delta_s\nu_j)_D = 2\nu^o_j \sqrt{\frac{2\ln 2 \, \kappa T_s}{M_s c^2}} \tag{3}$$

In Eq. 3, κ is Boltzmann's constant, T_s is the absolute temperature of the source, M_s is the molecular weight of the emitting molecule, and c is the speed of light.

In general, the frequency distribution of the absorption coefficient (k_{ν_j}) is given by (Ref. 6):

$$k_{\nu_j} = k_{\nu_j^o} \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{a'e^{-y^2}}{a'^2 + (\omega_j - y)^2} \, dy \tag{4}$$

where

$$a' = \frac{(\Delta_a\nu_j)_L}{(\Delta_a\nu_j)_D} \sqrt{\ln 2} \tag{5}$$

$$\omega_j = \frac{2(\nu_j - \nu^o_j)}{(\Delta_a\nu_j)_D} \sqrt{\ln 2} \tag{6}$$

and y is a dummy variable of integration. In Eq. 4, $k_{\nu_j^o}$ is the absorption coefficient at line center for Doppler conditions. In Eq. 5, $(\Delta_a\nu_j)_L$ is the Lorentz half-width (due to collision broadening) of the absorption line and is given by (Ref. 6):

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$$(\Delta_a \nu_j)_L = \frac{Z_L}{\pi} \tag{7}$$

where Z_L is the frequency of collisions between the absorbing molecules and the surrounding molecules which leads to broadening of the energy states of the absorbing molecules. The factor $(\Delta_a \nu_j)_D$ is the Doppler half-width of the absorption line and is given by

$$(\Delta_a \nu_j)_D = 2 \nu_j^o \sqrt{\frac{2 \ln 2 \, \kappa T_a}{M_a \, c^2}} \tag{8}$$

where T_a is the static temperature of the absorbing medium and M_a is the molecular weight of the absorbing molecules.

Equation 4 for k_{ν_j} can be shown to reduce to (Ref. 7):

$$k_{\nu_j} = k_{\nu_j^o} \, R\{\exp[-(\omega_j + ia')^2] \, \text{erfc} \, [-i\omega_j + a']\} \tag{9}$$

where R denotes the real part and $i = \sqrt{-1}$. It should be noted that, for low pressures and high temperatures, a' is very small and Eq. (9) reduces to

$$k_{\nu_j} = k_{\nu_j^o} \, e^{-\omega^2} \tag{10}$$

This is the Doppler case examined in Ref. 1.

Close examination of Eq. (9) shows that the absorption line half-width increases and the absorption coefficient at line center decreases as a' increases, as illustrated graphically in Fig. 1.

Equations (1), (2), and (4) can be combined to give the transmission of a single line through a medium:

$$T_j = I_{\nu_j^o}^c \int_o^\infty \exp \left\{ - \left[\frac{2(\nu - \nu_j^o)}{(\Delta_s \nu_j)_D} \sqrt{\ln 2} \right]^2 \right\} \exp \left\{ -\ell k_{\nu_j^o} \frac{1}{\pi} \int_{-\infty}^\infty \frac{a' e^{-y^2} dy}{a'^2 + (\omega_j - y)^2} \right\} d\nu \tag{11}$$

If there are other absorption lines which might contribute to the measured transmission of the jth line, Eq. (4) must be replaced by
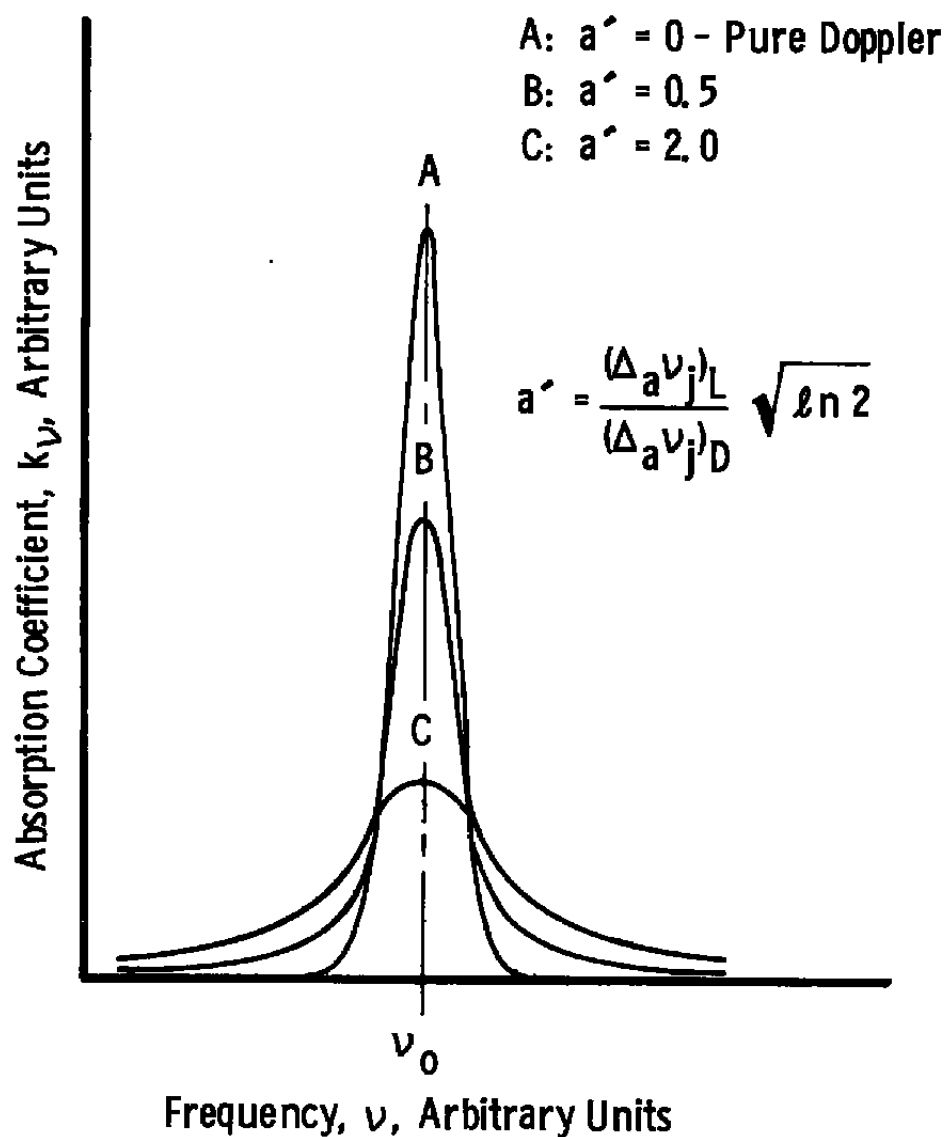
Figure 1. Illustration of spectral line shape for different values of the ratio of the pressure broadened half-width to the Doppler half-width.

$$k_\nu = \frac{1}{\pi} \sum_i k_{\nu_i^0} \int_{-\infty}^{\infty} \frac{a' e^{-y^2}}{a'^2 + (\omega_i - y)^2} \, dy \qquad (12)$$

where the summation is over all absorption lines, including the jth line, which have a finite value of the absorption coefficient contributing to absorption of the jth emission line. The transmission of the radiation in the jth emission line due to absorption by many lines is given by

$$T_j = I_{\nu_j^0}^0 \int_0^\infty \exp\left\{ -\left[\frac{2(\nu - \nu_j^0)}{(\Delta_s \nu_j)_D} \sqrt{\ell n\, 2} \right]^2 \right\} \exp\left\{ \frac{\ell}{\pi} \sum_i k_{\nu_i^0} \int_{-\infty}^\infty \frac{a' e^{-y^2} dy}{a'^2 + (\omega_i - y)^2} \right\} d\nu \qquad (13)$$

The total transmission $(\overline{T})$ in a particular frequency interval (e.g., bandpass of a spectrometer or interference filter) is given by summing over all the emission lines in that interval and results in the equation:

$$\overline{T}_{\Delta\nu} = \sum_j I_{\nu_j^0}^0 \int_0^\infty \exp\left\{ -\left[\frac{2(\nu - \nu_j^0)}{(\Delta_s \nu_j)_D} \sqrt{\ell n\, 2} \right]^2 \right\} \exp\left\{ -\frac{\ell}{\pi} \sum_i k_{\nu_i^0} \int_{-\infty}^\infty \frac{a' e^{-y^2} dy}{a'^2 + (\omega_i - y)^2} \right\} d\nu \qquad (14)$$

where the summation over j includes all emission lines which have components falling within the frequency interval of interest $(\Delta\nu)$. The transmissivity (t) or fractional transmission in a particular frequency interval $(\Delta\nu)$ is then given by

$$(15)$$

$$t_{\Delta\nu} = \frac{\sum_j I_{\nu_j^0}^0 \int_0^\infty \exp\left\{ -\left[\frac{2(\nu - \nu_j^0)}{(\Delta_s \nu_j)_D} \sqrt{\ell n\, 2} \right]^2 \right\} \exp\left\{ -\frac{\ell}{\pi} \sum_i k_{\nu_i^0} \int_{-\infty}^\infty \frac{a' e^{-y^2} dy}{a'^2 + (\omega_i - y)^2} \right\} d\nu}{\sum_j I_{\nu_j^0}^0 \int_0^\infty \exp\left\{ -\left[\frac{2(\nu - \nu_j)}{\Delta_s \nu_j)_D} \sqrt{\ell n\, 2} \right]^2 \right\} d\nu}$$

In order to carry out the evaluation of $t_{\Delta\nu}$, values of $k_{\nu_i^0}$ and a' must be determined for a particular medium and path.

2.2 RELATIONS BETWEEN ABSORPTION COEFFICIENT AND ABSORBING MEDIUM PROPERTIES

The absorption coefficient of a diatomic molecule for Doppler conditions at line center frequency $(k_{\nu_i^o})$ is given by (Ref. 5):

$$k_{\nu_i^o} = \frac{2e^2 \sqrt{\pi \, \ln 2}}{mc^2} \frac{N_{J''} f_{J'J''}}{(\Delta_a \nu_i)_D} \tag{16}$$

where e is the charge on an electron, c is the velocity of light, m is the mass of an electron, $f_{J'J''}$ is the oscillator strength of the appropriate absorption line, $N_{J''}$ is the number density of molecules in the lower energy state of the molecule corresponding to the ith line, J'' is the rotational quantum number of the lower energy state, and J' is the rotational quantum number of the upper energy state.

The number density of the lower energy state $(N_{J''})$ under equilibrium conditions is given by

$$N_{J''} = \frac{hc \, B_0 (2J'' + 1) \exp\left[-\frac{hc}{\kappa T_a} F(J'')\right]}{2 \kappa T_a} N_0 \tag{17}$$

where N_0 is the number density of the molecule of interest, B_0 is the rotational constant for the ground state, h is Planck's constant, κ is Boltzmann's constant, and $F(J'')$ is the rotational energy term for the lower rotational energy state.

The value for the oscillator strength $(f_{J'J''})$ is given by (Ref. 8):

$$f_{J'J''} = f_{v'v''} \frac{\nu_{J'J''}}{\nu_{v'v''}} \frac{S_{J''J'}}{2(2J'' + 1)(2S + 1)} \tag{18}$$

where $f_{v'v''}$ is the band oscillator strength, $\nu_{J'J''}$ is the frequency of the line of interest, $\nu_{v'v''}$ is the frequency of the band head, $S_{J''J'}$ is the normalized Hönl-London factor for the line of interest, and S is the spin quantum number. Combining Eqs. (16), (17), and (18) gives

$$k_{\nu_i^o} = \frac{e^2 \sqrt{\pi \, \ln 2} \, h \, B_0 \nu_{J'J''} f_{v'v''} S_{J''J'} N_0 \exp\left[-\frac{hc}{\kappa T_a} F(J'')\right]}{2(2S + 1) mc^2 \kappa T_a \nu_{v'v''} (\Delta_a \nu_i)_D} \tag{19}$$

13

For a particular spectral line of a given molecular species for which the various molecular parameters in Eq. (19) are known, values of $k_{\nu_i^*}$ can be calculated as functions of N_O and T_a.

For the (0, 0) γ-band of NO, Eq. (19) reduces to (Ref. 1):

$$k_{\nu_i^o} = 1.603 \times 10^{-14} \frac{\delta_{J'J''} N_o}{T_a^{3/2}} \exp\left[-1.4383 \, F(J'')/T_a\right] \qquad (20)$$

where the cgs system of units is used throughout

2.3 EXAMINATION OF THE BROADENING PARAMETER (a')

Equation (7) states that collisional broadening of a spectral absorption line depends on the collisional frequency of the absorbing molecules with the surrounding molecules. It can be shown from classical kinetic theory that the broadening collisional frequency (Z_L) for an absorbing molecule of molecular weight (M_a) is given by

$$Z_L = \sum_\ell Z_\ell = 2 \sum_\ell N_\ell \, \sigma_\ell^2 \, \sqrt{2\pi \kappa T_a \left(\frac{1}{M_\ell} + \frac{1}{M_a}\right)} \qquad (21)$$

where M_ℓ is the mass of the ℓth type of colliding molecule causing the broadening, N_ℓ is the concentration of the ℓth type of molecule, and σ_ℓ^2 is the effective collisional cross section for the broadening process by the ℓth type molecule.

Combining Eqs. (5), (7), (8), and (21) results in the equation,

$$a' = \frac{\lambda_j^o}{\sqrt{\pi}} \sum_\ell N_\ell \, \sigma_\ell^2 \, \sqrt{1 + \frac{M_a}{M_\ell}} \qquad (22)$$

where λ_j^o is the wavelength of the absorption line at line center and results from the fact that

$$\lambda_j^o = \frac{c}{\nu_j^o} \qquad (23)$$

By using the equation of state for a perfect gas, it can be shown that

$$N_\ell = 9.66 \times 10^{19} \frac{p_\ell}{T_a} \qquad (24)$$

where p_ℓ is the partial pressure of the ℓth type molecule in torr and T is in K. Combining Eqs. (22) and (24) results in

$$a' = \frac{5.45 \times 10^{19}}{T} \lambda_j^o \sum_{\ell} P_{\ell} \sigma_{\ell}^2 \sqrt{1 + \frac{M_a}{M_{\ell}}} \qquad (25)$$

For many cases, the foreign gas is composed of chiefly one constituent, and the concentration of the absorbing gas is relatively small. In such cases, self broadening is negligible, and Eq. (25) reduces to

$$a' = \left[5.45 \times 10^{19} \lambda_j \sigma^2 \sqrt{1 + \frac{M_a}{M_f}} \right] \frac{P_a}{T_a} \qquad (26)$$

or

$$a' = C_j \frac{P_a}{T_a} \qquad (27)$$

where σ^2 is the effective collisional cross section for the broadening process by the foreign gas, M_f is the mass of the foreign gas, and C_j is a constant for the jth line given by

$$C_j = 5.45 \times 10^{19} \lambda_j \sigma^2 \sqrt{1 + \frac{M_a}{M_f}} \qquad (28)$$

It is this constant (C_j) that must be determined experimentally.

3.0 DETERMINATION OF THE BROADENING PARAMETER (a') FOR THE NO MOLECULE IN THE PRESENCE OF N₂

The value of a is functionally dependent on pressure and temperature as shown by Eq. (27). To completely define a', the value of C_j must be determined experimentally. Although C_j depends on the wavelength of the spectral line of interest, for most spectral bands C_j may be considered a constant for all lines in the band and simply designated by C (i.e., λ_j changes by less than 0.1 percent throughout the (0, 0) γ-band of NO). In this section, the experimental determination of C_j for a few individual lines of the (0, 0) γ-band of NO and the determination of C for the entire, unresolved band will be described.

3.1 DESCRIPTION OF THE EXPERIMENTAL APPARATUS

The experimental apparatus consisted of a resonance gas discharge source lamp, a heated absorption cell, and two spectrometers. The arrangement of the apparatus is illustrated in Fig. 2.

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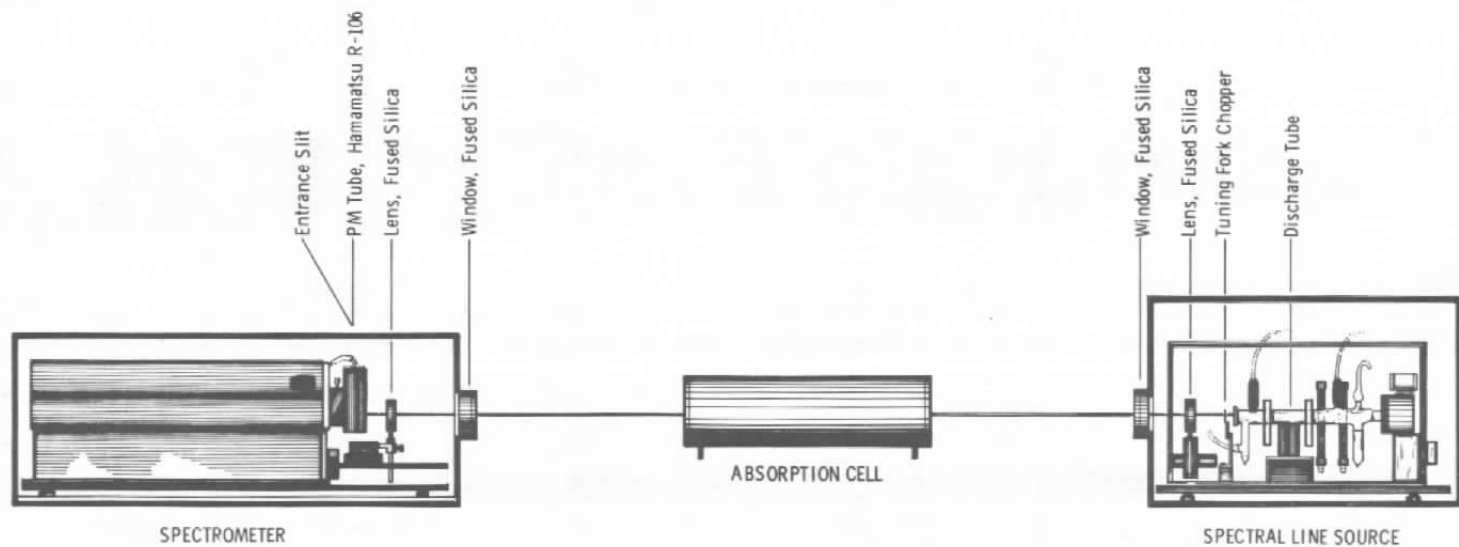
Figure 2. Schematic of experimental apparatus for resonance line absorption measurements.

3.1.1 Ultraviolet Spectrometers

A 1-m Jarrell-Ash grating spectrometer equipped with curved slits was used to obtain high resolution data. The grating has 1,180 lines/mm and was blazed for maximum reflection at 7,500 Å. All data taken with the 1-m spectrometer was in the second order of the spectrum. An RCA 1P28 photomultiplier tube with S-spectral response was used as the detector. The internal optics consisted of two fused silica lenses, each with an f-number of 4.4. The lenses were placed as shown in Fig. 2, so that parallel light was directed from the source through the absorbing gas and focused on the slit of the spectrometer. The 1-m spectrometer was operated with a physical slit width of $10\,\mu$, resulting in an equivalent slit width of 0.03 Å, which gives sufficient resolution to separate several lines in the γ-bands of NO (Ref. 3).

A 1/2-m Jarrell-Ash grating spectrometer equipped with curved slits was used to obtain low resolution band spectra. The grating had 2,360 lines/mm and was blazed for maximum reflection at 3,000 Å. The external optics and detector were identical to those used on the 1-m spectrometer. The 1/2-m spectrometer was operated with a physical slit width of $200\,\mu$, resulting in an equivalent slit width of 1.6 Å. No lines of NO γ-bands could be resolved using this slit width. The 1/2-m instrument, operated with the 200-μ slit width, has been used in lieu of the 1-m instrument for field measurements of the absorption of NO γ-band radiation (Ref. 4) because it is less susceptible to vibration and misalignment problems.

3.1.2 Absorption Cell

The absorption cell used in this research study was a specially designed 91.4-cm long by 10.2-cm-diam fused-silica tube with flat fused-silica end plates and 1/2-in. tubes for gas entry and exit (Fig. 3). The tube was enclosed in a copper sleeve which was wrapped with a Calrod[®] unit for heating purposes. A highly reflective aluminum sheet was wrapped around the heating unit, and the entire assembly was surrounded by three inches of insulation. The assembly was encased in a steel housing. Three-inch diameter holes were left in each end of the tube so that the light source could be directed through the cell and into the spectrometer.

The heating unit was connected to a temperature controller which controlled the temperature of the gas within the cell through the monitoring of strategically placed thermocouples. The temperature could

be varied between ambient and 1,000°F and controlled within an accuracy of ±1 percent. The pressure of the gas in the cell was measured by means of pressure transducers over a range of from 50 to 1,500 torr, with an accuracy of ±1 percent.

The gas system is shown schematically in Fig. 4. The absorber gases could be admitted to the cell and sealed off by valves or could be flowed continuously. In this experiment, the gases were admitted and sealed off. The gases used were mixtures of NO in N_2 which were supplied by Scott Research Corporation as calibration gases. Three mixtures were used: (1) 40 parts per million (ppm), (2) 100 ppm, or (3) 400 ppm of NO. The actual mixtures were determined to be 40, 99, and 395 ppm, using a gas chromatograph, with an accuracy of ±5 percent.

3.1.3 Resonance Lamp Source Characteristics

A schematic of the resonance lamp used as a line source is presented in Fig. 5. The source was run using a 12:3:1 mixture (by volume) of $(A:N_2:O_2)$ at approximately 5-torr pressure with an applied voltage of 2,800 v. Radiation emitted at the end of the water-cooled capillary tube was directed through the absorption cell and into the optics of the spectrometer (Fig. 2). The gas temperature in the capillary tube was maintained at approximately 320 K by the water-cooling jacket. It is assumed that the dominant broading mechanism under these conditions is due to the Doppler effect. The Doppler line width (Eq. (3)) for the lines of the (0, 0) γ-band of NO at 320 K is 0.0005 Å, so that the actual width of the lines is much smaller than the equivalent slit width of the spectrometer (0.03 Å). A spectrum of the (0, 0) band from the lamp in which many of the lines are resolved is given in Fig. 6. In order to employ the computational technique developed in Section 2.0 and the spectrometer simulation described in Ref. 1, it is necessary to define the relative intensity of each line in the band. By using all the resolved lines in the spectra of Fig. 6, a plot of the radiation intensity divided by the relative line strength versus the upper state energy (F_J') was made (Fig. 7). The upper state energy parameter varies from the energy at $J' = 1/2$ to the energy at $J' = 81/2$. A more complete discussion of the energy levels of the upper state for the (0, 0) γ-bands appears in Ref. 3.

In order to find the relative intensity of those lines that are not resolvable, it is necessary to use the curve in Fig. 7. For a particular line, the value of $I_{J'J''}/\delta_{J'J''}$ corresponding to its value of $F_{J'}$ is found from Fig. 7 and is then multiplied by the appropriate value of $\delta_{J'J''}$ resulting in a value of the relative intensity $(I_{J'J''})$ for the $J'J''$
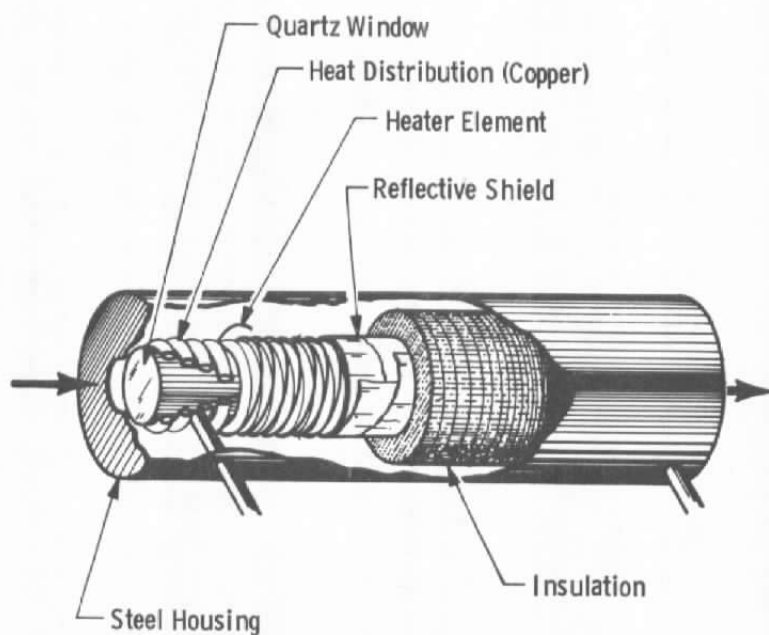
Figure 3. Diagram of heated absorption cell.
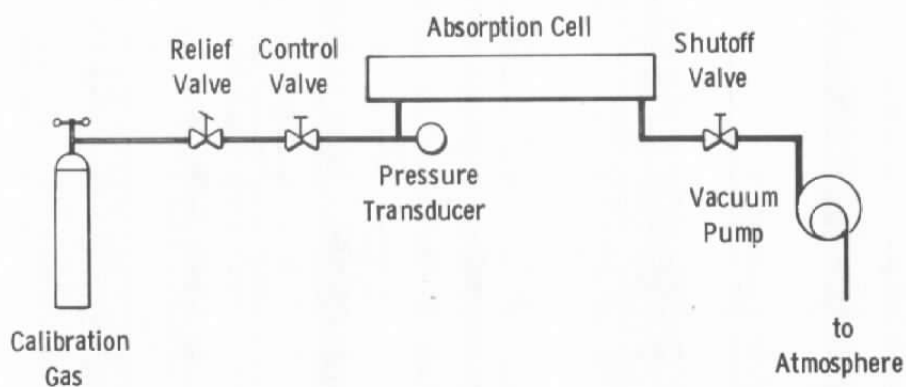
Figure 4. Schematic of gas handling system for heated absorption cell.
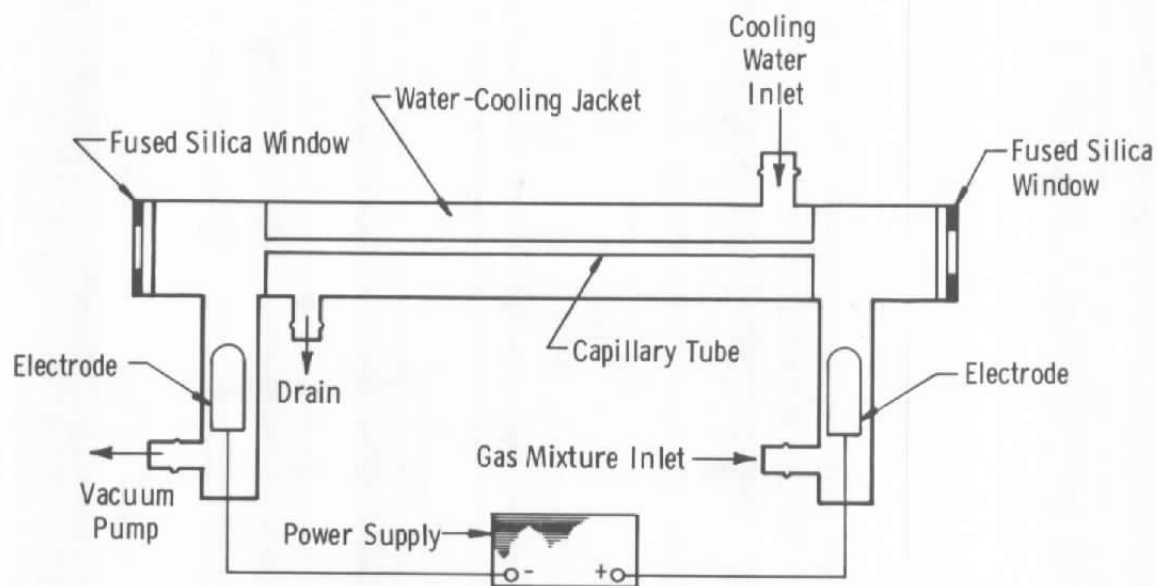
Figure 5. Diagram of resonance lamp used to produce narrow-line radiation.
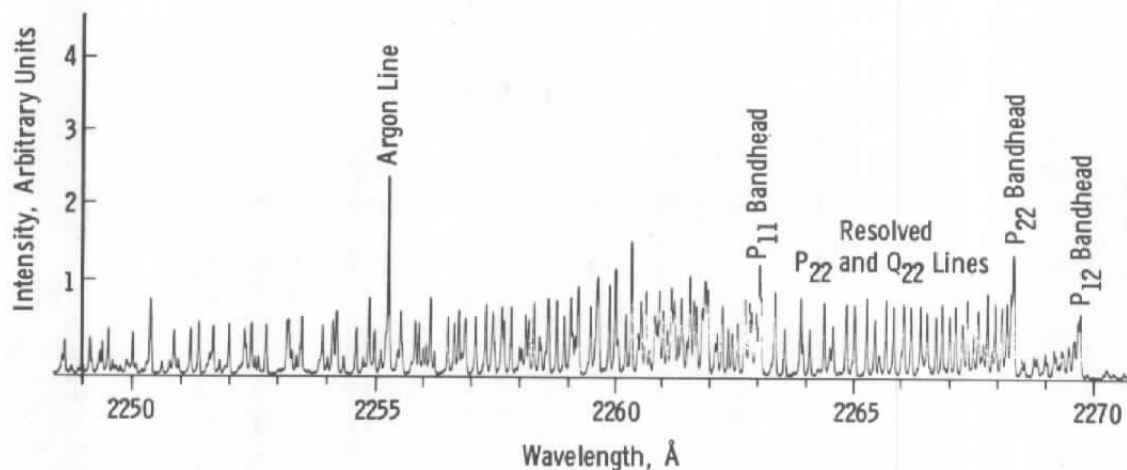
Figure 6. (0,0) band of the NO γ-system obtained from discharge tube containing a mixture of 12:3:1 (by volume) of A:N₂:O₂ at 8 torr with 2,800 v applied by use of 1-m spectrometer in second order (equivalent slit width, 0.03 Å).

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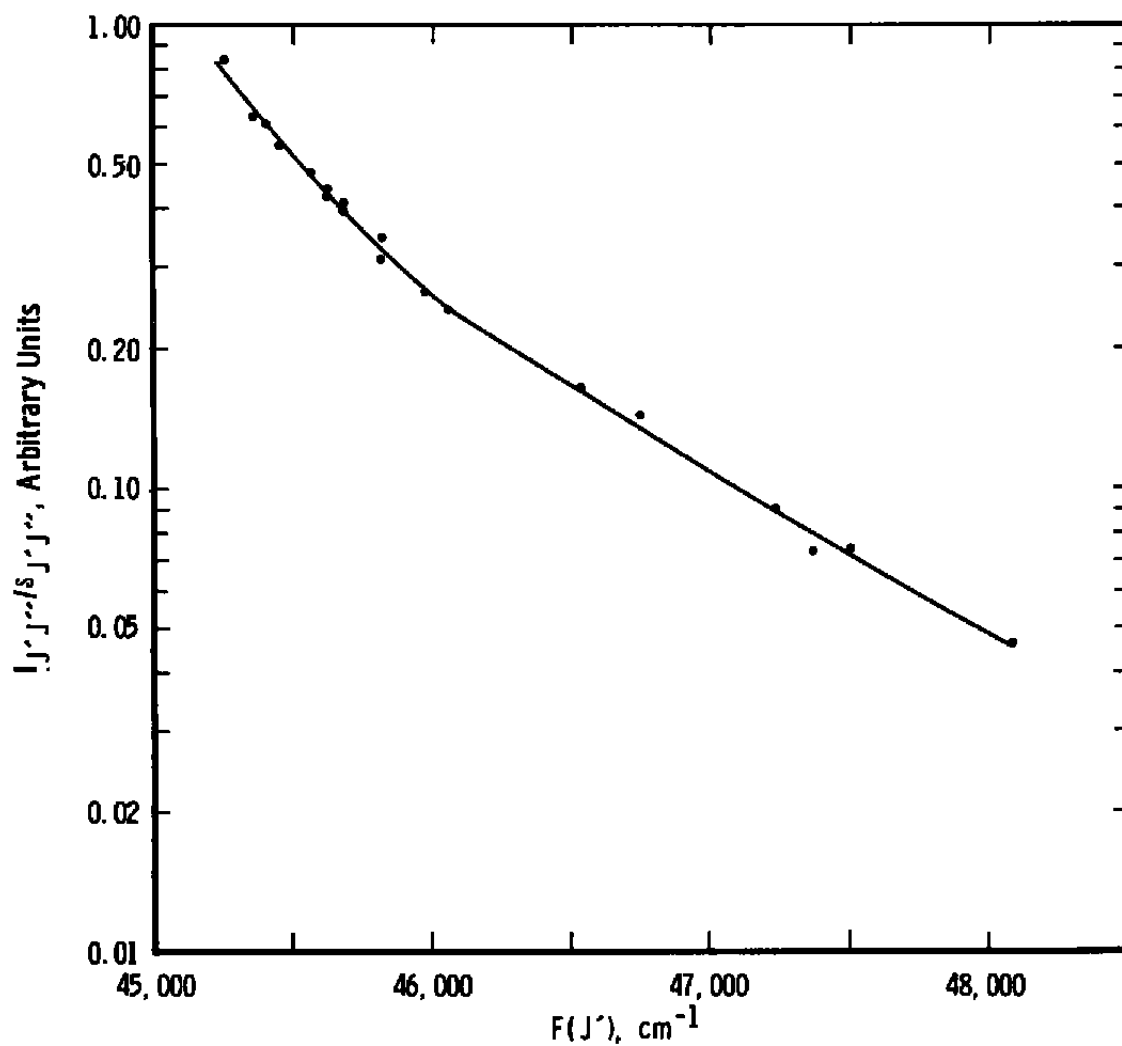
Figure 7. Population distribution of excited rotational states of the
$A^2\Sigma$ level of NO in a water-cooled discharge tube operated
at 8 torr with 2,800 v applied and containing 12:3:1 mixture
(by volume) of $A:N_2:O_2$.

line. Values for $\delta_{J'J''}$ are obtained from the formulas developed by Earls (Ref. 9) as given in Ref. 3. Experimental values of ν_j, as given by Deeszi (Ref. 10) were used in these calculations. The experimental values of ν_j are more accurate than can be calculated using the Hill and Van Fleck formula as discussed in Ref. 1. Values for I_{ν_j} used in the transmission equations (Eqs. (13), (14), or (15)) are thus calculated from the values of $I_{J'J''}/\delta_{J'J''}$ in Fig. 7.

The distributions of line intensities were measured several times during these experiments using pressures in the resonance lamp ranging from 5 to 15 torr with corresponding changes in the applied voltage and current. No measurable changes in the relative distribution of line intensities shown in Fig. 7 have been found, although the level of intensity may change considerably with the lamp operating conditions.

3.2 PROCEDURES AND RESULTS

The procedure for determining the value of C for NO consisted of the following steps:

(1) A series of laboratory spectral absorption measurements of the (0, 0) γ-band of NO were made for several partial pressures of NO and N_2 and for several gas temperatures. Several sets of high resolution data were taken using the 1-m spectrometer to measure the spectral transmission at the various conditions. A portion of the resolved spectrum for one of these tests is shown in Fig. 8 with no gas in the cell and with a mixture of NO and N_2 in the cell. For the case illustrated in Fig. 8, the number density of NO is 2.58×10^{15} molecules/cm^3, the pressure is 1.5 atm, and the temperature is 422 K. Several lines used to obtain values of a' are identified in Fig. 8. The transmissivity (t_j) for each of the lines was determined. Data comparable to that shown in Fig. 8 were obtained for three conditions in the absorption cell. Low resolution measurements were also made with the 1/2-m spectrometer in order to determine the transmission of the unresolved band. Example data for the band transmission are shown in Fig. 9 with the operating conditions stated on the figure. The transmissivity at the second band-head was determined from the data in Fig. 9. Unresolved band transmission data for the second band-head were obtained at 27

a. Optical path length for absorption ($N_o \ell = 0$)

b. Optical path length for absorption ($N_o \ell = 2.36 \times 10^{17}$ molecules/cm^2)
Figure 8. Example of transmission measurements for NO (0,0) γ-band, as obtained with a 1-m spectrometer having an equivalent slit width of 0.03 Å.

23
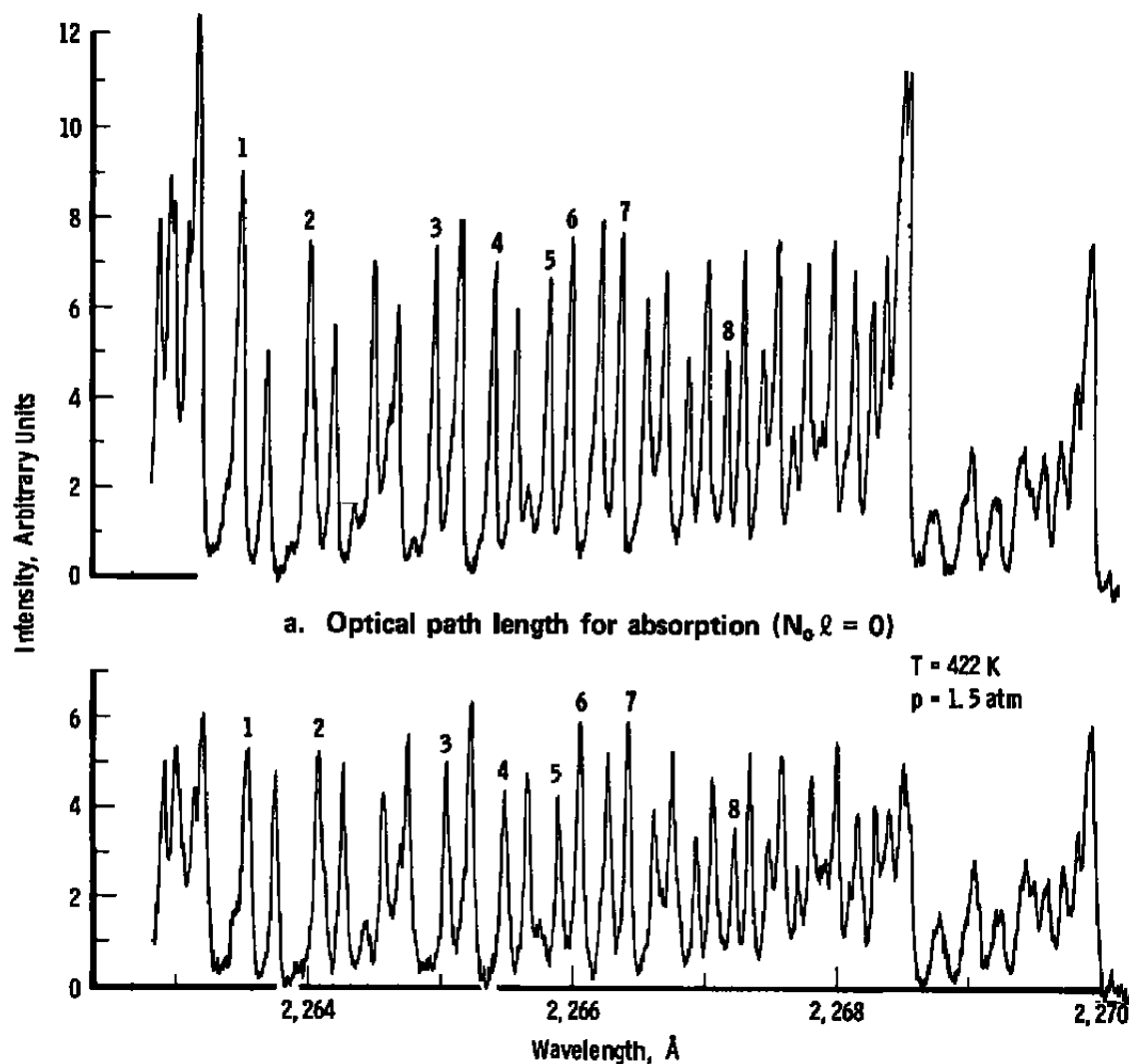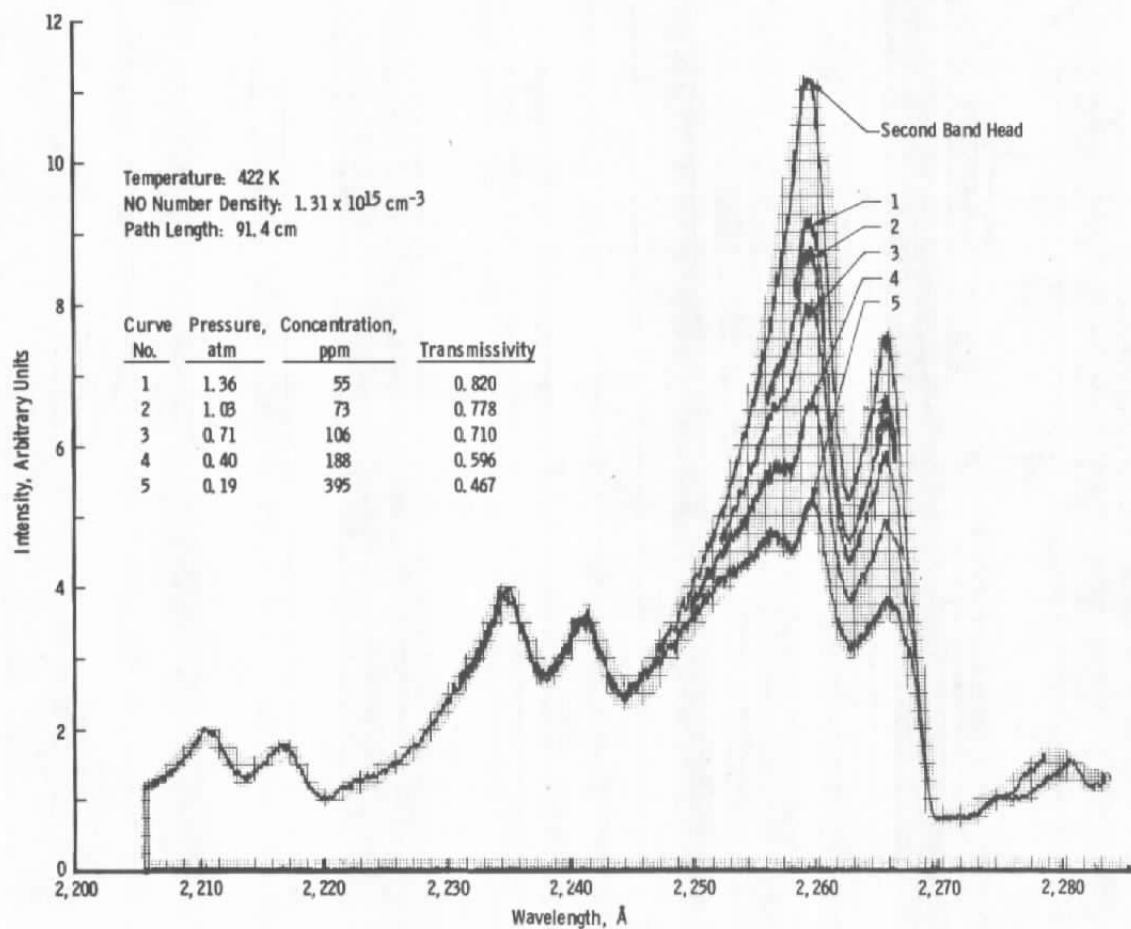
Figure 9. Example set of transmission measurements for NO (0,0) γ-band, as obtained with a 1/2-m spectrometer having an equivalent slit width of 1.6 Å.

conditions of pressure, temperature, and NO concentration in the cell.

(2) By using the computer simulation of spectra described in Ref. 1 and utilizing Eq. (14), a series of calculated transmitted spectra for many values of a′ was obtained for several values of NO concentration, temperature, and with the spectrometer slit width identical to that used in the laboratory experiments. An example synthetic spectrum for the high resolution simulation is shown in Fig. 10, and an example for the low resolution simulation is shown in Fig. 11. The computer program for spectral simulation is presented in Appendix A.

(3) By comparing the laboratory spectra taken at a given set of pressure, temperature, and concentration conditions in the absorption cell with the computer simulated spectra, which was calculated for the same conditions and at various values of a′, the value of a′ which best matches the experimental result was determined. The procedure is illustrated by comparing Fig. 8 with Fig. 10 and Fig. 9 with Fig. 11. The computed spectra led to values of transmission for varying values of a′, as illustrated in Fig. 12, which is taken from the second band-head transmission for various a′ values in Fig. 11. The values of a′ in Figs. 10 and 11 were the values which gave the best match between the measured and computed spectra. The values were chosen in this way so that the reader might make a direct comparison of the simulated and measured spectra. In practice, the a′ values for a particular experimental condition were obtained from plots like Fig. 12, which were obtained from simulated spectra over a range of arbitrarily selected values of a′.

The results obtained from the high resolution spectral absorption measurements are summarized in Table 1, and the results from the low resolution data are summarized in Table 2. For the high resolution data, eight individual lines were selected for determining the values of C_j. These lines are numbered in Table 2 to correspond to Figs. 8 and 10. For the low resolution data, the transmission at the second band-head as marked in Figs. 9 and 11 was used for determining the values of a′.
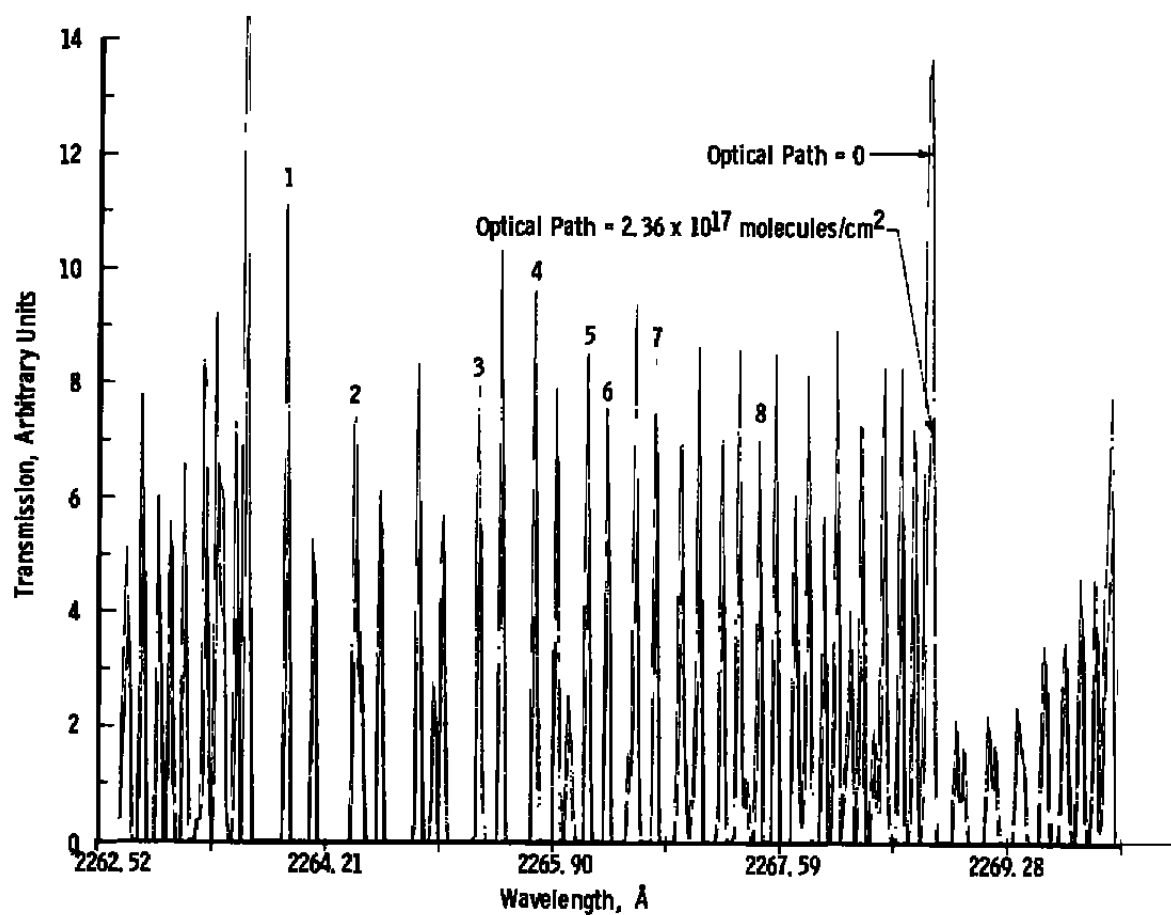
Figure 10. Example of computed transmission for NO (0,0) γ-band
for an equivalent spectral slit width of 0.03 Å and at
conditions corresponding to Fig. 8.
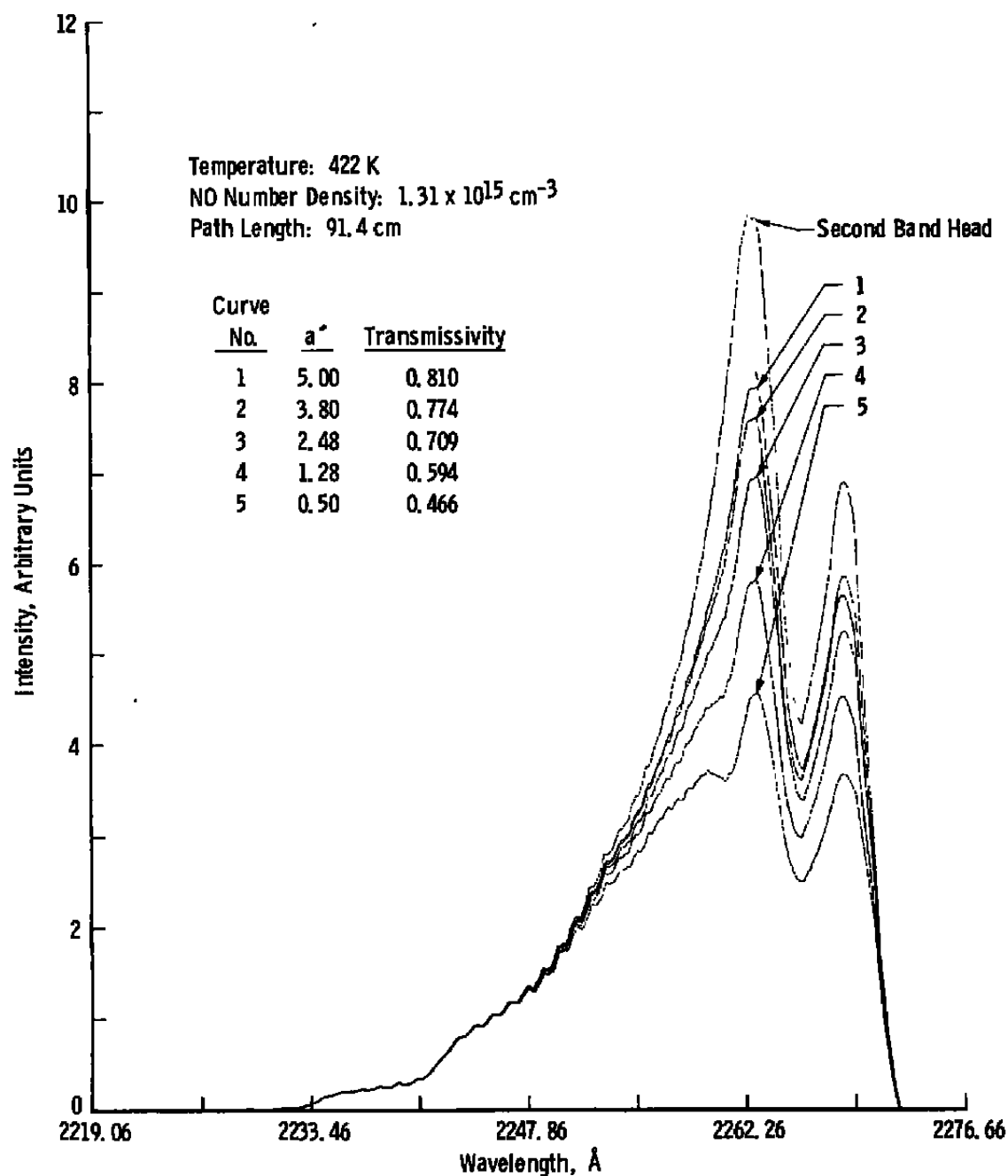
Figure 11. Example set of computed transmission for NO (0,0) γ-band
for an equivalent spectral slit width of 1.6 Å and at
conditions corresponding to Fig. 9.

27
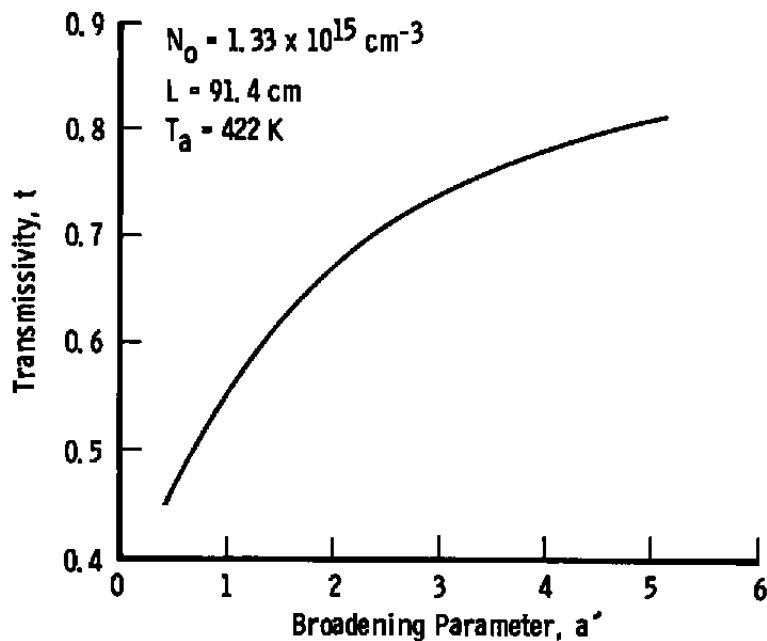
Figure 12. Calculated transmissivity (t) of the second band head of the (0,0) NO γ-band as a function of the line broadening parameter (a').

Table 1. Determination of Broadening Parameter (a') from Resolved Lines of the (0,0) Band of the NO γ-System

Line Number	Absorbing Medium Parameters			t	a'
	NO, Molecules/cm^3	Pressure, atm	Temperature, K		
1	2.58×10^{15}	1 500	422	0.84	4.4
2				0.73	4.6
3				0.70	4.5
4				0.67	4.4
5				0.66	4.4
6				0.85	4.6
7				0.82	4.5
8				0.76	4.6
1	10.32×10^{15}	1.500	422	0 19	4.5
2				0.28	4.6
3				0.25	4.6
4				0.21	4.0
5				0.21	4.3
6				0.51	4.9
7				0.45	4.8
8				0.27	4.1
1	1×10^{15}	0.102	296	0.65	0.8
2				0.66	0 7
3				0.54	0.7
4				0.52	0.5
5				0 51	0.5
6				0.84	0.5
7				0.78	0.6
8				0.59	0.7

Table 2. Determination of Broadening Parameter (a') from the Unresolved
(0,0) Band of the NO γ-System

Absorbing Medium Parameters			T, Second Band Peak	a'
NO, Molecules/cm^3	Pressure, atm	Temperature, K		
1.33 x 10^{15}	0.190	422	0.465	0.50
	0.395	422	0.591	1.28
	0.707	422	0.710	2.48
	1.034	422	0.777	3.80
7.52 x 10^{13}	0.721	744	0.977	1.00
	1.362	744	0.988	2.65
1.36 x 10^{14}	0.190	411	0.900	0.30
	0.395	411	0.942	1.18
	0.707	411	0.965	2.54
3.314 x 10^{14}	0.190	422	0.792	0.34
	0.395	422	0.870	1.26
	0.721	422	0.920	2.63
	1.034	422	0.936	3.70
2.75 x 10^{15}	0.395	422	0.323	1.00
	0.707	422	0.436	1.84
	1.034	422	0.526	2.74
	1.361	422	0.586	3.55
1.61 x 10^{15}	0.408	744	0.498	0.34
	0.721	744	9.658	1.21
	1.034	744	0.752	2.22
3.91 x 10^{15}	0.395	296	0.270	1.95
	0.707	296	0.330	2.75
	1.020	296	0.402	3.77
	1.350	296	0.468	5.18
1.89 x 10^{15}	0.190	296	0.370	1.03
	0.395	296	0.450	1.65
	0.707	296	0.600	3.35

The tabulated values of a' are plotted as a function of the ratio p/T in Fig. 13, and a straight line given by a least mean square fit is drawn through the points. The value of C in Eq. (27) (shown as C_j) is equal to the slope of the line in Fig. 12. For the (0, 0) γ-band of NO, C is found to be 1,270 ± 200 K/atm. From Eq. (28), the value of the optical cross section (σ^2) is found to be (9.5 ± 1.5) x 10^{-16} cm^2. The optical diameter is 3.5 ± 0.3 Å approximated by Thorsen and Badger in Ref. 2 from the experimental work carried out by Weber and Penner (Ref. 11).

4.0 DISCUSSION

The major use for the work reported herein is to determine calibration curves for the transduction of transmission measurements of NO γ-band radiation through media containing NO to the number density of NO in the media. Such calculations are used to extend laboratory calibrations at limited pressures and temperatures to a wider range of values; thus accurate values of the broadening parameter becomes a necessity. An application of the use of the calculations to a measurement situation is described in Ref. 12, where calibration curves are generated for absorption through the exhaust of a turbine engine burner at temperatures well above those possible in a laboratory absorption cell.

The uncertainty in values of a' projects the uncertainty in the final values of concentration determined from the γ-band absorption measurements. The estimated uncertainty in the values of a' given in Fig. 13 is about ±16 percent. When this value of uncertainty is used to determine the density of absorbers, the projected uncertainty in the density is about ±10 percent and constitutes the principal uncertainty in the resonance absorption technique for concentration measurements through uniform media. A more accurate value of a' would correspondingly reduce the possible uncertainty in measuring the concentration of NO. However, experimental errors in measurements of this nature would probably limit the uncertainty to no better than ±5 percent so that pursuit of a better value for the constant C is probably not warranted for purposes of measurement.

The experimental work from which the determination of a' was made utilized mixtures of NO in N_2. Thus, the foreign broadening gas is N_2. The question arises as to whether other gases which might
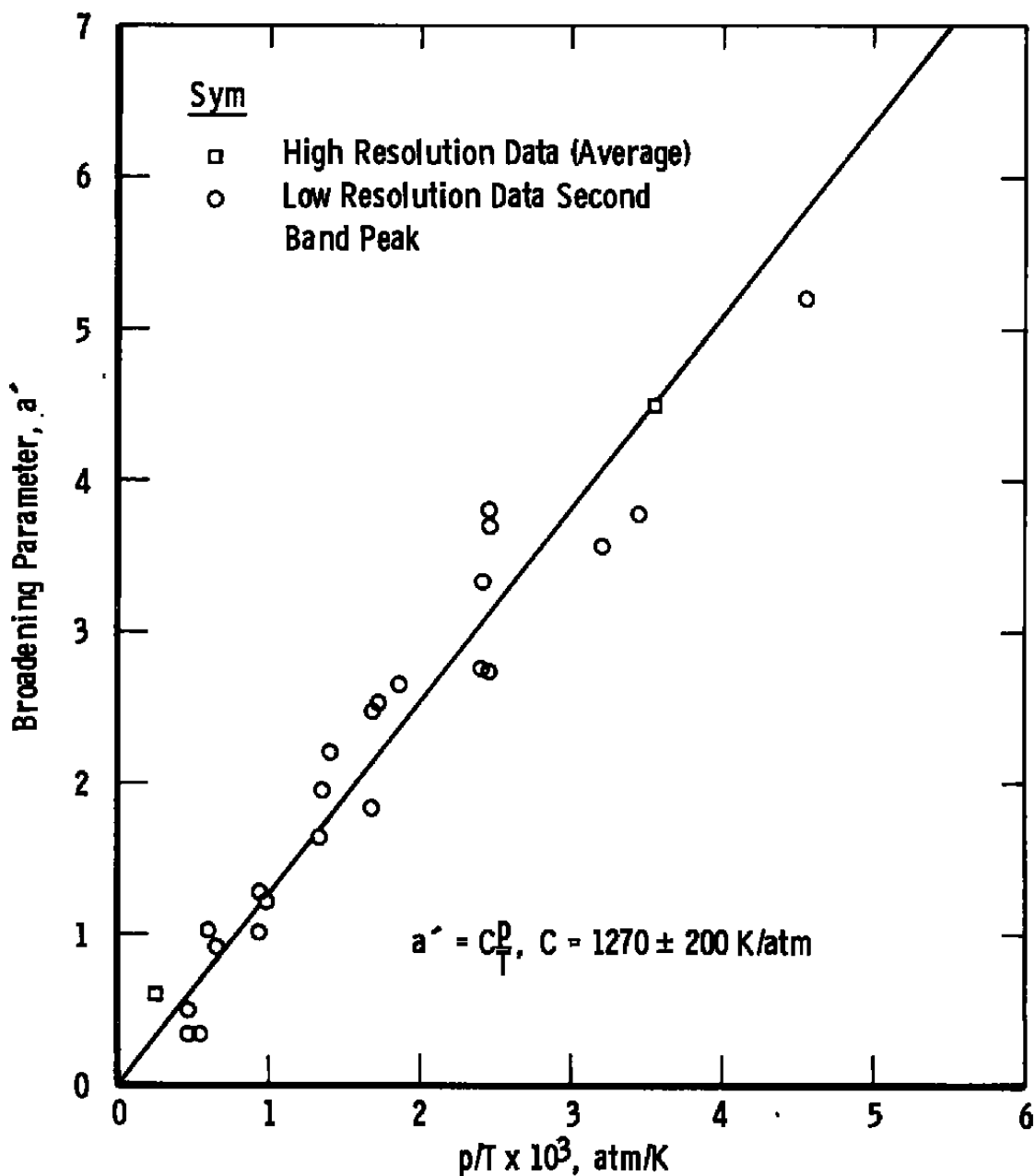
Figure 13. Values of the spectral broadening parameter (a′) as
a function of p/T for the (0,0) γ-band of NO as
obtained by comparing experimental data with
computed data.

be found in combustion gas streams, such as CO_2, H_2O, CO, etc., might have significantly different broadening cross sections. Based on the results presented in Ref. 5 for CO, the broadening cross section for NO is not believed to be significantly different for other molecules than for N_2. Experience with measurements in absorption cells located in sample lines in which measurements of NO concentration made by other means agreed well with the values obtained by the absorption technique (Ref. 12) also gives confidence to the universality of the broadening parameter with different molecules.

The indirect method of determining the broadening parameter used in this study is believed to be a valid alternative to the use of high resolution spectroscopy to measure line shapes and thus determine the parameter directly. However, the method requires the use of a good model for the radiation source and for the absorbing media, and a high speed digital computer to accomplish the complex numerical calculations.

Finally, a significant result of the work reported herein is the improved value of the effective cross section (or diameter) for collisional broadening of the ground state energy levels of NO. The value of the effective broadening collision diameter (3.5 ± 0.3 Å) determined in this work offers considerable improvement in uncertainty over the best known previous estimate of Thorsen and Badger (Ref. 2) of 3.8 ± 1 Å.

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APPENDIX A
COMPUTER PROGRAM FOR THE CALCULATION AND SIMULATION OF THE
NO (0,0) γ-BAND SPECTRA TRANSMITTED THROUGH
AN ABSORBING MEDIUM

The computer program included in this appendix was developed
to calculate the transmission of a band of spectral lines from a partic-
ular molecule through an absorbing medium containing the same molec-
ular species. The approach may be used for any molecule, but the
line structure and angular momentum coupling are so different for
each species that a separate program is usually needed for each
molecular species. In this appendix, the computational procedure is
described for the NO molecule.

DESCRIPTION

The program is separated into two steps. Step 1 records all
input data and computes the transmission of the radiation due to each
source line. Step 2 processes these data and generates the simulated
spectrometer output signal. The program is currently being run on
the IBM 370-165 computer; X-Y plotter data are presented on the
CALCMP 765 plotter.

PROGRAM STEP 1

The first program step is divided into four parts:

Part 1 — Input Data

Part 1 contains the various COMMON and DIMENSION statements
for the program. If more than 500 emission lines are to be considered,
a modification of the program would be necessary. Values of $\Delta\lambda$, a',
T_a, T_s, and ℓ and various plot control parameters are input. Details
of the input data and format are discussed in the following paragraph.

Part 2 — Spectral Line Calculation

Cards identifying each emission-line to be considered are read.
For each line, the rotational energy of the upper electron state $F(J')$
is computed via SUBROUTINE FUPPER, and the rotational energy of

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the lower rotation state $F(J'')$ is computed in SUBROUTINE FLOWER. The Hönl-London factor is then computed in SUBROUTINE HONNUM. The value of $I_{\nu_j}^o$ is found by interpolation from Fig. 7. The curve in Fig. 7 is an input to the program.

For the $(0, 0)$ γ-Band of NO, the values of $k_{\nu_i}^o$ are given by Eq. (20) and are computed in Part 2.

Part 3 — Line-By-Line Transmission Calculation

In Part 3, the transmission (Eq. (13)) is evaluated for each line. Since k_ν is a function of ν, many time-consuming evaluations of k_ν are apparent. In fact, if there are n nodes used in the numerical integration, then nm^2 evaluations are required where m is the number of lines being considered. If the program variable ALLOW is set to zero, the program will sum over all the lines, i.e.,

$$\sum_i k_{\nu_i} = \sum_{i=1}^m k_{\nu_i} \tag{A-1}$$

To save time (although at the expense of some accuracy), another option is available. This option is selected by setting ALLOW > 0. By considering the jth spectral line, the sum $\sum_i k_{\nu_i}$ is written as:

$$\sum_i k_{\nu_i} \approx \sum_{i=j}^{j+j_u} k_{\nu_i} + \sum_{i=j-1}^{j-j_\ell} k_{\nu_i} \tag{A-2}$$

Note that the index in the second sum decreases. The indices j_u and j_e are chosen so that the contributions of the $(j + j_u)$th and $(j - j_e)$th lines are as small as desired. The exact criterion used is

$$\left| \frac{k_{\nu_{j+j_u}}}{\sum_{i=j}^{j-j_u} k_{\nu_i}} \right| < \text{ALLOW} \tag{A-3}$$

and

$$\left| \frac{k_{\nu_{j-j_u}}}{\sum_{i=j-1}^{j-j_\ell} k_{\nu_i}} \right| < \text{ALLOW} \tag{A-4}$$

In effect, only those lines in a chosen neighborhood of ν_j^o are considered.

If a′ = 0, no collision broadening is considered and k_{ν_i} is calculated from Eq. (10). If a′ > 0, then k_{ν_i} must be given by Eq. (A-4).

Subroutine WFUNC evaluates the function

$$R\{\exp\left[-(\omega_j + ia')^2\right] \text{erfc}\left[-i\omega_j + a'\right]$$

which is contained in Eq. (9) and leads to the determination of k_{ν_j}. The subsequent evaluation of the integral in Eq. (13) is done numerically using the trapezoidal rule.

Part 4 — Data Storage

This part writes program control data as well as wavenumber and source line transmission data onto a disc file for passage to Step 2.

PROGRAM STEP 2

Step 2 performs the plotting functions of the program. The mathematical and physical considerations are presented in detail in Ref. 1.

The program first reads in the various control parameters from Step 1. Then, the first set of values of ν_j and $\overline{T}_j$ are read in. These data correspond to the first value of N_0 supplied to Step 1. All following curves will be plotted according to the scale factor determined from the initial case. Generally, the case $N_0 = 0$ (no absorption) is calculated first, and all other plots are referenced to this case (Fig. 1).

If IPLOT1 = 1, then zero slit width plots are produced (Fig. 2).

If IPLOT2 = 1, a separate plot is produced for each value of N_0 as well as the final combined plot.

The conglomerate spectral profile is constructed as follows: A line with a height proportional to the spectral intensity is drawn at $\lambda_i + 1/2\,\Delta\lambda_x'$ for each spectral line and a triangular slit function of base width $2\Delta\lambda_x'$ is constructed about that line. To arrive at the conglomerate profile, the contributions from each line at a given value of λ are simply added.

PROGRAM VARIABLE DESCRIPTION

The following variables are used in the program:

Mathematical Symbol	Program Variable	Usage
$\tilde{T}_j$	TJ(J)	Transmission of spectral line, j
ν_j°	WO(J)	Center wavenumber of jth spectral line
$(\Delta_s \nu_j)_D$	DWJ	Doppler width at half maximum intensity of jth spectral line
$(\Delta_a \nu_j)_D$	DWL	Doppler width at half maximum absorption coefficient $k_{\nu_j^\circ}$ of the absorption line
$I_{\nu_j^\circ}$	E(J)	Intensity of source spectral line
$I_{\nu_j^\circ}^\circ$	EO(J)	Intensity of source spectral line at center wavenumber
k_{ν_i}	CAY(I)	Absorption coefficient for the ith line
ℓ	EL	Absorption path length
a'	AP	Collisional broadening parameter
T_s	TE	Source gas temperature, K
T_a	TA	Absorber gas temperature, K
$\Delta\lambda$	SLIT	Equivalent slit width
N_o	ENO	Total number density
V'	IVU	Upper vibrational state
V''	IVL	Lower vibrational state
J''	RJPP	Lower rotational state

Mathematical Symbol	Program Variable	Usage
	W(I)	Nodes for numerical integration (Eq. (1))
	NUP	Upper spin state
	NLO	Lower spin state
	BRANCH	Line branch designation
	IPLOT 1	For zero slit width plots, set IPLOT1 = 1 otherwise = 0
	IPLOT 2	For separate N_O plots, set IPLOT2 = 1, otherwise = 0
	YHGT	Maximum height of spectral plots, in.
	DELPLT	Scale for abscissa of spectral plots, A°/in.
$S_{J''J'}$	S(J)	Hönl-London factor for jth line
$F(J')$	FU	Rotational energy of the upper electron state
$F(J'')$	FL(J)	Rotational energy of the lower rotational state
	ALLOW	Relative error (see Eq. (10))
m	NLINES	Number of emission lines

DATA INPUT

All data is input to Step 1.

<u>CARDS 1</u>   FORMAT (2F10.0)

Column 1 F(J')   Column 11 $(I_{\nu_j^\circ}/\delta_{J''J}')$

The first cards expected by the program are values of $(I_{\nu_j^\circ}/\delta_{J''J}')$ versus F_{u_j}, one data pair per card. The cards should be arranged in order of increasing F_{u_j}. A blank card must follow the final data card of this group. The data for the source lamp used in the measurements shown in this report are given in Table A-1.

<u>CARD 2</u>   TITLE CARD   FORMAT (20A4)

This card should contain any title information the user wishes to use for plot identification.

<u>CARD 3</u>   DELPLT   FORMAT (F10.0)

<u>CARD 4</u>   SLIT   FORMAT (F10.0)

<u>CARD 5</u>   AP   FORMAT (F10.0)

<u>CARD 6</u>   TA   FORMAT (F10.0)

<u>CARD 7</u>   TE   FORMAT (F10.0)

<u>CARD 8</u>   EL   FORMAT (F10.0)

<u>CARD 9</u>   YHGT   FORMAT (F10.0)

<u>CARD 10</u>   IPLOT1   FORMAT((I1)

<u>CARD 11</u>   IPLOT2   FORMAT (I1)

<u>CARDS 12</u>   FORMAT (3X, A1, 2I1, 1X, F4.0, 1X, F11.0)

These cards are those which describe the spectral lines to be considered.

COLUMN 4   BRANCH (P, Q, or R)   FORMAT A1

,COLUMN 5   NUP   FORMAT I1

.   COLUMN 6   NUPP   FORMAT I1

COLUMN 8-11   RJPP   F4.0

COLUMN 13-23   WO   F11.0

These cards must be arranged in order of increasing wavenumber WO. A blank card must follow the last line description card. The data for the NO (0, 0) γ-Band are given in Table A-2.

CARDS 13   FORMAT (F10.0)

These cards contain the values of ENO to be considered. All plots will be scaled to the plot representing the first value of ENO in this group.

SAMPLE CASE

The case to be considered here is the (0, 0) NO γ-band with collisional broadening considered. The following values will be used:

$$a' = 1.5$$
$$T_a = 420 \text{ K}$$
$$T_e = 320 \text{ K}$$
$$\ell = 91 \text{ cm}$$
$$\Delta\lambda = 1.6 \text{ Å}$$
$$N_o = 0., 1 \times 10^{15}, 1 \times 10^{16} \text{ cm}^{-3}$$
$$YHGT = 10 \text{ in.}$$
$$DELPLT = 6 \text{ Å/in.}$$

The equations and constants used for computing the upper and lower energy states and the Hönl-London factors are discussed in Ref. 3 and are repeated here for completeness.

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For the upper state (SUBROUTINE FUPPER),

$$F' = T'_e + G' + F'_n \qquad n = 1,2$$

where

$$T'_e = 43965.7 \ cm^{-1}$$

$$G' = \omega'_e(v' + 1/2) - \omega_e x'_e(v' + 1/2)^2$$

where

$$\omega'_e = 2374.8 \ cm^{-1}$$
$$\omega_e x'_e = 16.46 \ cm^{-1}$$

$$F'_1 = B'_v(J' + 1/2)(J' - 1/2) + D'_v(J' + 1/2)^2(J' - 1/2)^2$$
$$F'_2 = B'_v(J' + 1/2)(J' + 3/2) + D'_v(J' + 1/2)^2(J' - 3/2)^2$$
$$B'_v = B'_e - \alpha'_e(v' + 1/2)$$

where

$$B'_e = 1.9977 \ cm^{-1}$$
$$\alpha'_e = 0.0198 \ cm^{-1}$$
$$D'_v = -6.2 \times 10^{-6} \ cm^{-1}$$

For the lower state (SUBROUTINE FLOWER),

$$F'' = T''_e + G'' + F''_n \qquad n = 1, 2$$
$$T''_e = G'' = 0$$

$$F''_1 = B''_v[(J'' + 1/2)^2 - 1 - u] + D''_v J''^4$$
$$F''_2 = B''_v[(J'' + 1/2)^2 - 1 + u] + D''_v(J'' + 1)^4$$

where

$$u = \left[(J'' + 1/2)^2 - Y_v\left(1 - \frac{Y_v}{4}\right)\right]^{1/2}$$
$$Y_v = A/B''_v$$

and

$$A = 124.2 \ cm^{-1}$$
$$B''_v = B''_e - \alpha''_e(v'' + 1/2)$$
$$B''_e = 1.7046 \ cm^{-1}$$
$$\alpha''_e = 0.0178 \ cm^{-1}$$
$$D_v = -4.8 \times 10^{-6} \ cm^{-1}$$

The Hönl-London factors are given in Table A-3.

The emission lines being considered can be read from the
data card listing which follows.   The plots produced by this case are
shown in Fig. A-1.   Many other calculations as well as comparisons
between actual and computed spectra are presented in Ref. 1.
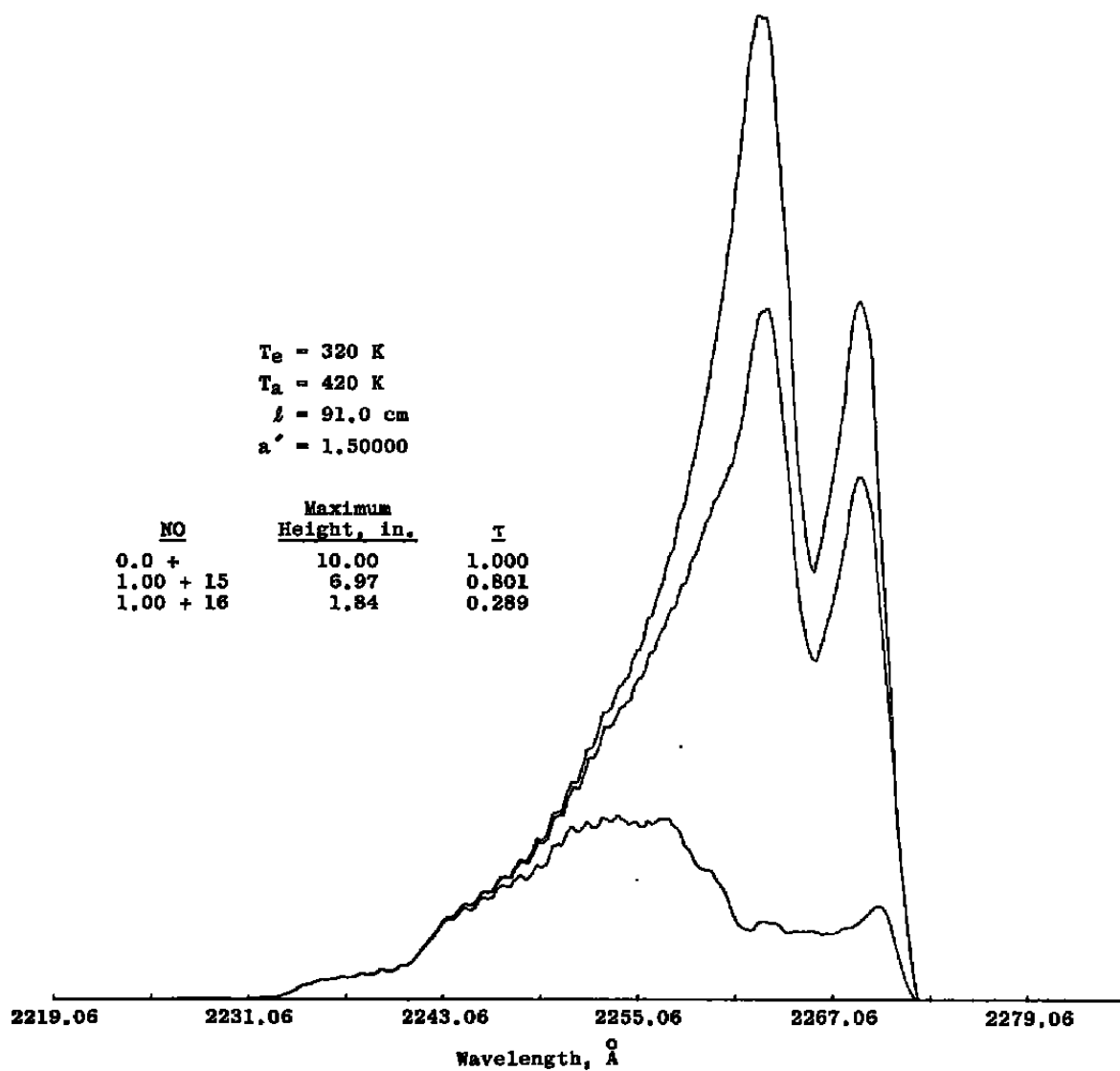
Figure A-1. Spectral test case.

Table A-1. Data Cards for Sample Case

┌─Column 1

45100.	1.25	48600.	.0218
45200.	.92	48700.	.0198
45300.	.68	48800.	.018
45400.	.54	48900.	.0165
45500.	.45	49000.	.015
45600.	.39	49100.	.0138
45700.	.33	49200.	.0126
45800.	.28	49300.	.0115
45900.	.255	49400.	.0105
46000.	.23	49500.	.0097
46100.	.208	49600.	.0088
46200.	.19	49700.	.0081
46300.	.175	49800.	.0074
46400.	.158	49900.	.0068
46500.	.145	50000.	.0062
46600.	.1325	50100.	.0056
46700.	.12	50200.	.0052
46800.	.11	50300.	.0047
46900.	.1	50400.	.0043
47000.	.092	50500.	.0039
47100.	.084	50600.	.0036
47200.	.077	50700.	.0033
47300.	.07	50800.	.003
47400.	.064		
47500.	.058		
47600.	.053		
47700.	.049		
47800.	.044		
47900.	.041		
48000.	.037		
48100.	.034		
48200.	.031		
48300.	.0285		
48400.	.026		
48500.	.0238		

Table A-2. Spectra Test Case

Blank Card
SPECTRA TEST CASE
6.
1.6
1.5
420.
320.
91. ┌─Branch (Column 4)
10. │ ┌─NUP (Column 5)
0   │ │ ┌─NUPP (Column 6)
0   │ │ │ ┌─RJPP (Column 8-11)

P12(10.5)	44052.03	
P12(11.5)	44052.03	
P12(9.5)	44052.03	
P12(12.5)	44052.78	
P12(8.5)	44052.78	
P12(13.5)	44054.22	
P12(7.5)	44054.22	
P12(14.5)	44056.16	
P12(6.5)	44056.49	
P12(15.5)	44058.33	
P12(5.5)	44058.80	
P12(16.5)	44061.30	
P12(4.5)	44061.77	
P12(17.5)	44064.66	
P12(3.5)	44065.40	
P12(18.5)	44068.69	
P12(2.5)	44069.60	
P12(19.5)	44073.21	
P12(1.5)	44074.26	
P22(3.5)	44077.58	
P22(4.5)	44077.95	
P22(2.5)	44077.95	
Q12(4.5)	44077.95	
Q12(2.5)	44077.95	
P12(20.5)	44078.59	
P22(5.5)	44078.59	
P22(1.5)	44078.59	
Q12(5.5)	44078.59	
Q12(1.5)	44078.59	
P22(6.5)	44080.32	
Q12(6.5)	44080.32	
P22(7.5)	44082.33	
Q12(7.5)	44082.33	
P12(21.5)	44084.33	
P22(8.5)	44084.83	
Q12(8.5)	44084.83	
Q22(1.5)	44086.15	

R12(1.5)	44086.15	
P22(9.5)	44087.98	
Q12(9.5)	44087.98	
Q22(2.5)	44089.56	
R12(2.5)	44089.56	
P12(22.5)	44090.28	
P22(10.5)	44091.56	
Q12(10.5)	44091.56	
Q22(3.5)	44093.39	
R12(3.5)	44093.39	
P22(11.5)	44095.70	
Q12(11.5)	44095.70	
R22(1.5)	44096.82	
P12(23.5)	44097.18	
Q22(4.5)	44097.68	
R12(4.5)	44097.68	
P22(12.5)	44100.45	
Q12(12.5)	44100.45	
Q22(5.5)	44102.72	
R12(5.5)	44102.72	
P12(24.5)	44104.59	
P22(13.5)	44105.72	
Q12(13.5)	44105.72	
R22(2.5)	44105.72	
Q22(6.5)	44108.17	
R12(6.5)	44108.17	
P22(14.5)	44111.50	
Q12(14.5)	44111.50	
P12(25.5)	44112.34	
R22(3.5)	44113.52	
Q22(7.5)	44114.15	
R12(7.5)	44114.15	
P22(15.5)	44117.84	
Q12(15.5)	44117.84	
P12(26.5)	44120.71	
Q22(8.5)	44120.71	
R12(8.5)	44120.71	
R22(4.5)	44121.52	
P22(16.5)	44124.74	
Q12(16.5)	44124.74	
Q22(9.5)	44127.68	
R12(9.5)	44127.68	
P12(27.5)	44129.98	
R22(5.5)	44130.42	
P22(17.5)	44132.16	
Q12(17.5)	44132.16	
Q22(10.5)	44135.31	
R12(10.5)	44135.31	

Table A-2. Continued

P12(28.5)	44140.13		P11(1.5)	44194.29
P22(18.5)	44140.13		R22(11.5)	44194.93
Q12(18.5)	44140.13		P12(33.5)	44195.91
R22(6.5)	44140.13		Q11(2.5)	44197.98
Q22(11.5)	44143.44		P21(2.5)	44197.98
R12(11.5)	44143.44		Q11(3.5)	44197.98
P22(19.5)	44148.68		P21(3.5)	44197.98
Q12(19.5)	44148.68		Q11(1.5)	44197.98
P12(29.5)	44149.83		P21(1.5)	44197.98
R22(7.5)	44149.83		P22(24.5)	44199.21
Q22(12.5)	44152.17		Q12(24.5)	44199.21
R12(12.5)	44152.17		P11(17.5)	44199.21
P22(20.5)	44157.73		Q11(4.5)	44199.21
Q12(20.5)	44157.73		P21(4.5)	44199.21
P12(30.5)	44160.46		Q11(0.5)	44199.21
R22(8.5)	44160.46		P21(0.5)	44199.21
Q22(13.5)	44161.32		Q11(5.5)	44200.13
R12(13.5)	44161.32		P21(5.5)	44200.13
P22(21.5)	44167.31		Q11(6.5)	44202.36
Q12(21.5)	44167.31		P21(6.5)	44202.36
Q22(14.5)	44171.19		Q22(17.5)	44203.49
R12(14.5)	44171.19		R12(17.5)	44203.49
R22(9.5)	44171.19		R11(0.5)	44203.49
P11(9.5)	44176.85		Q21(0.5)	44203.49
P11(8.5)	44176.85		P11(18.5)	44204.96
P22(22.5)	44177.28		Q11(7.5)	44204.96
Q12(22.5)	44177.28		P21(7.5)	44204.96
P11(10.5)	44177.28		R11(1.5)	44206.03
P11(7.5)	44177.28		Q21(1.5)	44206.03
P11(11.5)	44178.53		R22(12.5)	44207.81
P11(6.5)	44178.53		Q11(8.5)	44208.38
P11(12.5)	44180.58		P21(8.5)	44208.38
P11(5.5)	44180.58		R11(2.5)	44209.69
Q22(15.5)	44181.38		Q21(2.5)	44209.69
R12(15.5)	44181.38		R21(0.5)	44210.69
R22(10.5)	44183.02		P22(25.5)	44211.21
P11(13.5)	44183.02		Q12(25.5)	44211.21
P11(4.5)	44183.02		P11(19.5)	44211.21
P12(32.5)	44184.08		Q11(9.5)	44212.25
P11(14.5)	44186.07		P21(9.5)	44212.25
P11(3.5)	44186.07		R11(3.5)	44213.81
P22(23.5)	44188.16		Q21(3.5)	44213.81
Q12(23.5)	44188.16		Q22(18.5)	44215.46
P11(15.5)	44189.80		R12(18.5)	44215.46
P11(2.5)	44189.80		Q11(10.5)	44217.00
Q22(16.5)	44192.18		P21(10.5)	44217.00
R12(16.5)	44192.18		R21(1.5)	44217.60
P11(16.5)	44194.29		P11(20.5)	44217.73

Table A-2. Continued

R11(4.5)	44218.55	R11(10.5)	44260.93
Q21(4.5)	44218.55	Q21(10.5)	44260.93
R22(13.5)	44220.78	R21(6.5)	44261.79
Q11(11.5)	44222.24	P22(29.5)	44264.24
P21(11.5)	44222.24	Q12(29.5)	44264.24
P22(26.5)	44223.95	R22(16.5)	44264.24
Q12(26.5)	44223.95	Q11(17.5)	44266.44
R11(5.5)	44223.95	P21(17.5)	44266.44
Q21(5.5)	44223.95	Q22(22.5)	44268.65
R21(2.5)	44225.14	R12(22.5)	44268.65
P11(21.5)	44225.26	R11(11.5)	44269.92
Q22(19.5)	44228.00	Q21(11.5)	44269.92
R12(19.5)	44228.00	P11(26.5)	44271.53
Q11(12.5)	44228.00	R21(7.5)	44272.49
P21(12.5)	44228.00	Q11(18.5)	44275.98
R11(6.5)	44230.23	P21(18.5)	44275.98
Q21(6.5)	44230.23	P22(30.5)	44278.96
P11(22.5)	44233.24	Q12(30.5)	44278.96
R21(3.5)	44233.31	R22(17.5)	44278.96
R22(14.5)	44234.47	R11(12.5)	44279.65
Q11(13.5)	44234.47	Q21(12.5)	44279.65
P21(13.5)	44234.47	P11(27.5)	44282.69
P22(27.5)	44236.86	Q22(23.5)	44283.28
Q12(27.5)	44236.86	R12(23.5)	44283.28
R11(7.5)	44236.86	R21(8.5)	44283.28
Q21(7.5)	44236.86	Q11(19.5)	44286.10
Q22(20.5)	44241.13	P21(19.5)	44286.10
R12(20.5)	44241.13	R11(13.5)	44290.12
P11(23.5)	44241.68	Q21(13.5)	44290.12
Q11(14.5)	44241.68	P22(31.5)	44294.38
P21(14.5)	44241.68	Q12(31.5)	44294.38
R21(4.5)	44242.11	R22(18.5)	44294.38
R11(8.5)	44244.30	P11(28.5)	44294.38
Q21(8.5)	44244.30	R21(9.5)	44295.79
R22(15.5)	44249.10	Q11(20.5)	44296.87
Q11(15.5)	44249.10	P21(20.5)	44296.87
P21(15.5)	44249.10	Q22(24.5)	44298.56
P22(28.5)	44250.17	R12(24.5)	44298.56
Q12(28.5)	44250.17	R11(14.5)	44301.17
P11(24.5)	44251.31	Q21(14.5)	44301.17
R11(9.5)	44252.05	P11(29.5)	44306.57
Q21(9.5)	44252.05	Q11(21.5)	44308.22
R21(5.5)	44252.05	P21(21.5)	44308.22
Q22(21.5)	44254.52	R21(10.5)	44308.22
R12(21.5)	44254.52	P22(32.5)	44309.89
Q11(16.5)	44257.54	Q12(32.5)	44309.89
P21(16.5)	44257.54	R22(19.5)	44311.13
P11(25.5)	44260.93	R11(15.5)	44312.82

Table A-2. Continued

Q21(15.5)	44312.82	Q21(20.5)	44380.21
Q22(25.5)	44314.35	R21(15.5)	44380.21
R12(25.5)	44314.35	R22(23.5)	44382.31
P11(30.5)	44319.69	Q22(29.5)	44382.93
Q11(22.5)	44320.28	R12(29.5)	44382.93
P21(22.5)	44320.28	Q11(27.5)	44389.23
R21(11.5)	44321.38	P21(27.5)	44389.23
R11(16.5)	44325.12	P11(35.5)	44393.03
Q21(16.5)	44325.12	R11(21.5)	44395.56
P22(33.5)	44326.20	Q21(21.5)	44395.56
Q12(33.5)	44326.20	R21(16.5)	44396.60
R22(20.5)	44328.22	P22(37.5)	44397.04
Q22(26.5)	44330.62	Q12(37.5)	44397.04
R12(26.5)	44330.62	Q22(24.5)	44401.45
P11(31.5)	44332.92	R12(24.5)	44401.45
Q11(23.5)	44332.92	R22(24.5)	44401.45
P21(23.5)	44332.92	Q11(28.5)	44404.77
R21(12.5)	44335.22	P21(28.5)	44404.77
R11(17.5)	44337.97	P11(36.5)	44409.50
Q21(17.5)	44337.97	R11(22.5)	44411.51
P22(34.5)	44343.01	Q21(22.5)	44411.51
Q12(34.5)	44343.01	R21(17.5)	44413.05
R22(21.5)	44345.86	P22(38.5)	44416.27
Q11(24.5)	44345.86	Q12(38.5)	44416.27
P21(24.5)	44345.86	Q22(31.5)	44420.73
Q22(27.5)	44347.45	R12(31.5)	44420.73
R12(27.5)	44347.45	R22(25.5)	44421.02
P11(32.5)	44347.45	Q11(29.5)	44421.02
R21(13.5)	44349.51	P21(29.5)	44421.02
R11(18.5)	44351.46	P11(37.5)	44426.61
Q21(18.5)	44351.46	R11(23.5)	44428.01
Q11(25.5)	44359.81	Q21(23.5)	44428.01
P21(25.5)	44359.81	R21(18.5)	44430.56
P22(35.5)	44360.38	P22(39.5)	44435.89
Q12(35.5)	44360.38	Q12(39.5)	44435.89
P11(33.5)	44361.81	Q11(30.5)	44437.77
R22(22.5)	44363.61	P21(30.5)	44437.77
Q22(28.5)	44365.00	Q22(32.5)	44440.23
R12(28.5)	44365.00	R12(32.5)	44440.23
R21(14.5)	44365.00	R22(26.5)	44441.26
R11(19.5)	44365.55	P11(38.5)	44444.40
Q21(19.5)	44365.55	R11(24.5)	44445.05
Q11(26.5)	44374.12	Q21(24.5)	44445.05
P21(26.5)	44374.12	R21(19.5)	44448.65
P11(34.5)	44377.09	Q11(31.5)	44455.09
P22(36.5)	44378.49	P21(31.5)	44455.09
Q12(36.5)	44378.49	Q22(33.5)	44460.45
R11(20.5)	44380.21	R12(33.5)	44460.45

Table A-2. Concluded

R22(27.5)	44462.07		Q21(31.5)	44581.73
P11(39.5)	44462.71		R21(26.5)	44591.53
R11(25.5)	44462.71		Q22(39.5)	44593.46
Q21(25.5)	44462.71		R12(39.5)	44593.46
R21(20.5)	44467.16		Q11(38.5)	44593.46
Q11(32.5)	44473.15		P21(38.5)	44593.46
P21(32.5)	44473.15		R22(33.5)	44598.17
Q22(34.5)	44481.26		R11(32.5)	44603.58
R12(34.5)	44481.26		Q21(32.5)	44603.58
R11(26.5)	44481.26		R21(27.5)	44614.41
Q21(26.5)	44481.26		Q11(39.5)	44615.72
R22(28.5)	44483.40		P21(39.5)	44615.72
R21(21.5)	44486.41		R22(34.5)	44622.97
Q11(33.5)	44491.75		R11(33.5)	44626.16
P21(33.5)	44491.75		Q21(33.5)	44626.16
R11(27.5)	44500.09		R21(28.5)	44637.85
Q21(27.5)	44500.09		R22(35.5)	44648.22
Q22(35.5)	44502.61		R11(34.5)	44649.12
R12(35.5)	44502.61		Q21(34.5)	44649.12
R22(29.5)	44505.24		R21(29.5)	44661.86
R21(22.5)	44506.13		R11(35.5)	44672.76
Q11(34.5)	44510.92		Q21(35.5)	44672.76
P21(34.5)	44510.92		R22(36.5)	44673.94
R11(28.5)	44519.47		R21(30.5)	44686.59
Q21(28.5)	44519.47		R11(36.5)	44697.12
Q22(36.5)	44524.55		Q21(36.5)	44697.12
R12(36.5)	44524.55		R22(37.5)	44700.02
R21(23.5)	44526.75		R21(31.5)	44711.69
R22(30.5)	44527.76		R11(37.5)	44722.14
Q11(35.5)	44530.67		Q21(37.5)	44722.14
P21(35.5)	44530.67		R22(38.5)	44727.04
R11(29.5)	44539.74		R21(32.5)	44737.46
Q21(29.5)	44539.74		R11(38.5)	44747.37
Q22(37.5)	44546.76		Q21(38.5)	44747.37
R12(37.5)	44546.76		R22(39.5)	44754.43
R21(24.5)	44547.80		R21(33.5)	44763.28
R22(31.5)	44550.89		R11(39.5)	44773.43
Q11(36.5)	44550.89		Q21(39.5)	44773.43
P21(36.5)	44550.89		R21(34.5)	44789.81
R11(30.5)	44560.38		R21(35.5)	44818.26
Q21(30.5)	44560.38		R21(37.5)	44874.81
Q22(38.5)	44569.96		R21(38.5)	44904.54
R12(38.5)	44569.86		R21(39.5)	44934.51
R21(25.5)	44569.86		Blank Card	
Q11(37.5)	44571.93			
P21(37.5)	44571.93		0.0	
R22(32.5)	44574.03		.000E15	
R11(31.5)	44581.73		.000E16	

TABLE A-3
HÖNL-LONDON FACTORS FOR $^2\Sigma \rightarrow {}^2\pi$ TRANSITIONS
INTERMEDIATE BETWEEN HUND'S CASES (a) AND (b)

$$R_{22} = \frac{(2J''+1)^2 + (2J''+1)[Y(Y-4) - (2J''+1)^2]^{-\frac{1}{2}}(4J''^2 + 4J'' + 1 - 2Y)}{8(J''+1)}$$

$$Q_{22} = \frac{(2J''+1)[(4J''^2 + 4J'' - 1) + \{Y(Y-4) + (2J''+1)^2\}^{-\frac{1}{2}}(8J''^3 + 12J''^2 - 2J'' + 1 - 2Y)]}{8J''(J''+1)}$$

$$P_{22} = \frac{(2J''+1)^2 + (2J''+1)[Y(Y-4) + (2J''+1)^2]^{-\frac{1}{2}}(4J''^2 + 4J'' - 7 + 2Y)}{8J''}$$

$$R_{12} = \frac{(2J''+1)^2 - (2J''+1)[Y(Y-4) + (2J''+1)^2]^{-\frac{1}{2}}(4J''^2 + 4J'' - 7 + 2Y)}{8(J''+1)}$$

$$Q_{12} = \frac{(2J''+1)[(4J''^2 + 4J'' - 1) - \{Y(Y-4) + (2J''+1)^2\}^{-\frac{1}{2}}(8J''^3 + 12J''^2 - 2J'' - 7 + 2Y)]}{8J''(J''+1)}$$

$$P_{12} = \frac{(2J''+1)^2 - (2J''+1)[Y(Y-4) + (2J''+1)^2]^{-\frac{1}{2}}(4J''^2 + 4J'' + 1 - 2Y)}{8J''}$$

$$R_{11} = \frac{(2J''+1)^2 + (2J''+1)[Y(Y-4) + (2J''+1)^2]^{-\frac{1}{2}}(4J''^2 + 4J'' - 7 + 2Y)}{8(J''+1)}$$

$$Q_{11} = \frac{(2J''+1)[(4J''^2 - 4J'' - 1) + \{Y(Y-4) + (2J''+1)^2\}^{-\frac{1}{2}}(8J''^3 + 12J''^2 - 2J'' - 7 + 2Y)]}{8J''(J''+1)}$$

$$P_{11} = \frac{(2J''+1)^2 + (2J''+1)[Y(Y-4) + (2J''+1)^2]^{-\frac{1}{2}}(4J''^2 + 4J'' + 1 - 2Y)}{8J''}$$

$$R_{21} = \frac{(2J''+1)^2 - (2J''+1)[Y(Y-4) + (2J''+1)^2]^{-\frac{1}{2}}(4J''^2 + 4J'' + 1 - 2Y)}{8(J''+1)}$$

$$Q_{21} = \frac{(2J''+1)[(4J''^2 + 4J'' - 1) - \{Y(Y-4) + (2J''+1)^2\}^{-\frac{1}{2}}(8J''^3 + 12J''^2 - 2J'' + 1 - 2Y)]}{8J''(J''+1)}$$

$$P_{21} = \frac{(2J''+1)^2 - (2J''+1)[Y(Y-4) + (2J''+1)^2]^{-\frac{1}{2}}(4J''^2 + 4J'' - 7 + 2Y)}{8J''}$$

where $Y = A/B_v$

THE PROGRAM

```
IV G LEVEL  21              MAIN           DATE = 75178         09/06/45
      C
      C**********************************************************************
      C PART1     PART1     PART1     PART1     PART1     PART1     PART1     PART1
      C**********************************************************************
      C
            REAL*4 KO
            INTEGER*4 P,G,R,ELANK
            INTEGER*4 BRANCH
            DIMENSION S(500),FL(500),WC(500),EO(500)
            DIMENSION HEADS(20)
            DIMENSION KO(500)
            DATA P/'P'/,Q/'Q'/,R/'R'/
            DATA BLANK/' '/
            COMMON/PAREM/CONST1,CONST2,CCNST3,WO,EO,KO,NLINES
            DIMENSION W(500),E(500),CAY(500),OAT(500),EJ(500),TJ(500)
            CALL ERRSET(208,256,-1,1)
            ALLOW=.001
            CALL FUNC(XDUM)
            LIR2=2
            IVU=0
            IVL=0
            READ(5,366)HEADS
        366 FORMAT(20A4)
            READ(5,36)DELPLT
            READ(5,36)SLIT
            ULAM=SLIT
            READ(5,36)AP
            READ(5,36)TA
            READ(5,36)TE
            READ(5,36)EL
            READ(5,36)YHGT
            READ(5,700)IPLOT1
            READ(5,700)IPLOT2
        700 FORMAT(2I1)
         37 FORMAT(11,2F10.0)
            C1=.801550-14/TA**(3.00/2.00)
            C1=C1*2.00
            C2=-1.438360D/TA
            CONST1=-2.D0*DSQRT(DLGG(2.D0))
            CONST2=1.3C7D-74 SQRT(TE)
            CONST3=1.3C7D-74 SQRT(TA)
            CONST4=3.E-7*SQRT(TE)
            WRITE(6,87)HEADS,AP
         87 FORMAT(1H1,20X,20A4,10X,3HA*=,F7.4)
      C
      C**********************************************************************
      C PART2     PART2     PART2     PART2     PART2     PART2     PART2     PART2
      C**********************************************************************
      C
            J=1
        749 READ(5,1)BRANCH,NUP,NLC,RJPP,WC(J)
            IF(BRANCH.EQ.BLANK)GO TO 2
            JPP=RJPP
          1 FORMAT(JX,A1,I1,I1,1X,F4.0,1X,F11.0)
            IF(BRANCH.EQ.P)GO TO 1C
            IF(BRANCH.EQ.Q)GO TC 2C
```

```
      CALL FUPPER(IVU,NUP,JPP+1,FU)
      CALL MONNUM(IVU,IVL,NUP,NLO,JPP+1,JPP,3,S(J))
      GO TO 100
 36   FORMAT(4F10.0)
 20   CALL FUPPER(IVU,NUP,JPP ,FU)
      CALL MONNUM(IVU,IVL,NUP,NLC,JPP,JPP,2,S(J))
      GO TO 100
 10   CALL FUPPER(IVU,NUP,JPP-1,FU)
      CALL MONNUM(IVU,IVL,NUP,NLC,JPP-1,JPP,1,S(J))
 100  CALL FLOWER(IVL,NLC,JPP,FL(J))
      EO(J)=S(J)*FUNC(FU)
      WRITE(6,101)J,BRANCH,NUP,NLC,JPP,FU,FL(J),WO(J),S(J),EO(J)
 101  FORMAT(2X,I3,2X,A1,I1,I1,'(',I2,')','FU=',D16.8,5X,'FL=',D16.8,
     *5X,'WO=',D16.8,5X,'SJ=',D16.8,5X,'EOJ=',D16.8)
      J=J+1
      GO TO 749
 2    CONTINUE
      NLINES=J-1
 800  READ(5,36,END=800)ENU
      DO 69 I=1,NLINES
      B=C1*S(I)* EXP(C2*FL(I))
      KO(I)=B*ENU
 69   CONTINUE
C
C**************************************************************************
C-PART3    PART3    PART3    PART3    PART3    PART3    PART3    PART3
C**************************************************************************
C
      ISAVE=1
      NINT=40
      NP1=NINT+1
      TAUTOP=0.D0
      TAUBOT=0.D0
      DO 200 J=1,NLINES
      DWJ=CONST2*WO(J)
      DELTAW=CONST4*WO(J)
      AZJ=WO(J)-DELTAW
      BZJ=WO(J)+DELTAW
      DIST=BZJ-AZJ
      DEL=DIST/NINT
      DO 700 I=1,NP1
      W(I)=AZJ+(I-1)*DEL
      E(I)=EO(J)* EXP(-((W(I)-WO(J))*CONST1/DWJ)**2)
      IF(ENU.EQ.0.)GO TO 67447
      JLEFT=0
      SUML=0.
      SUMR=0.
      II=J
 1108 DWL=CONST3*WO(II)
      IF(AP.EQ.0.)GO TO 1100
      DETA=-CONST1*(W(I)-WO(II))/DWL
      CALL BFUNC(DETA,AP,TERM,DLWS)
      GO TO 1101
 1100 TERM=EXP(-((W(I)-WO(II))*CONST1/DWL)**2)
 1101 CONTINUE
      TNEW=KO(II)*TERM
```

```
        IF(JLEFT.EQ.1)GO TO 1109
        SUMR=SUMR+TNEW
        IF(WO(II).GT.W(I).AND.TNEW.EQ.0.)GO TO 1107
        IF(II.EQ.NLINES)GO TO 1107
        IF(WO(II).LT.BZJ)GO TO 33550
        IF(ABS(TNEW/SUMR).LE.ALLCW)GO TO 1107
33550   CONTINUE
        II=II+1
        GO TO 1108
 1107   JLEFT=1
        II=J-1
        IF(J.EQ.1)GO TO 7013
        GO TO 1108
 1109   CONTINUE
        SUML=SUML+TNEW
        IF(WO(II).LT.W(I).AND.TNEW.EQ.0.)GO TO 7013
        IF(II.EQ.1)GO TO 7013
        IF(WO(II).GT.AZJ)GO TO 33551
        IF(ABS(TNEW/SUML).LE.ALLCW)GO TO 7013
33551   CONTINUE
        II=II-1
        GO TO 1108
 7013   CONTINUE
        GO TO 7000
87447   SUML=0.
        SUMR=0.
 7000   CAY(I)=SUML+SUMR
        SUM1=0.00
        SUM2=0.00
        DEL2=DEL/2.00
        DO 9000 I=1,NP1
 9000   OAT(I)=E(I)* EXP(-CAY(I)*EL)
        DO 9001 I=1,NINT
        SUM1=SUM1+DEL2*(OAT(I)+OAT(I+1))
 9001   SUM2=SUM2+DEL2*(E(I)+E(I+1))
        EJ(J)=SUM2
        TJ(J)=SUM1
        TAUTOP=TAUTOP+TJ(J)
        TAUBUT=TAUBUT+EJ(J)
  200   CONTINUE
C
C******************************************************************************
C PART4     PART4     PART4     PART4     PART4     PART4     PART4     PART4
C******************************************************************************
C
        TAU=TAUTOP/TAUBUT
        ALPHA=1.00-TAU
        WRITE(L,848) TA,TL,ENG,EL,TAU,ALPHA
  848   FORMAT(//,5X,'TA=',D16.8,5X,'TE=',D16.8,5X,'AC=',D16.8,5X,'L=',
       *D16.8,5X,/,5X,'TAU=',D16.8,5X,'ALPHA=',D16.8)
        WRITE(20)SLIT,PLTMIN,PLTMAX,DELPLT,DLAM,YMGT,NLINES,END,
       *TL,TA,EL,IPLOT1,IPLOT2
       *,LIN2,AP
       *,TAU
       *,HEADS
        DO 5431 I=1,NLINES
```

```
        LKT=NLINES-I+1
 9431   WRITE(20)NO(LKT),TJ(LKT)
        GO TO 200
  800   ENDFILE 20
        REWIND 20
        STOP
        END
```

.

.

.

```
       FUNCTION FUNC(X).
       DIMENSION XDATA(100),YDATA(100)
       DATA IRST/0/
       IF(IRST.EQ.0)GO TO 1
       IF(X.LT.XDATA(1))GO TO 200
       DO 10 I=1,NP1
       IF(XDATA(I).LE.X.AND.XDATA(I+1).GE.X)GO TO 20
   10 CONTINUE
       FUNC=(YDATA(NP)-YDATA(NP1))*(X-XDATA(NP))/(XDATA(NP)-XDATA(NP1))+Y
      +DATA(NP)
       RETURN
   20 FUNC=(YDATA(I+1)-YDATA(I))/(XDATA(I+1)-XDATA(I))*(X-XDATA(I))
      +*YDATA(I)
       RETURN
  200 FUNC=(YDATA(2)-YDATA(1))*(X-XDATA(1))/(XDATA(2)-XDATA(1))+YDATA(1)
       RETURN
    1 DO 100 I=1,1000
       READ(5,2)XDATA(I),YDATA(I)
    2 FORMAT(8F10.0)
       IF(XDATA(I).EQ.0.0D0)GO TO 3
  100 CONTINUE
    3 CONTINUE
       NP=I-1
       NP1=NP-1
       IRST=1
       RETURN
       END
```

```
      SUBROUTINE FUPPER(V,M,JINDEX,F)
C
C     SUBROUTINE FUPPER CALCULATES THE ROTATIONAL ENERGY OF THE UPPER
C     ELECTRON STATE FOR A GIVEN VIBRATIONAL STATE(V), A GIVEN SPIN
C     STATE(M), AND A GIVEN ROTATIONAL STATE(J)
C
      INTEGER V
      REAL*4 J
      J=JINDEX+.5
      T=43905.7
      WE=2J74.6
      WEXE=16.46
      BE=1.5977
      ALPHAE=.0158
      DV=-6.2E-6
      BV=BE-ALPHAE*(V+.5)
      GO TO(1,2),M
    1 FN=BV*(J+.5)*(J-.5)+DV*(J+.5)**2*(J-.5)**2
      GO TO 3
    2 FN=BV*(J+.5)*(J+1.5)+DV*(J+.5)**2*(J+1.5)**2
    3 CONTINUE
      G=WE*(V+.5)-WEXE*(V+.5)**2
      F=T+G+FN
      RETURN
      END
```

```
        SUBROUTINE FLOWER(V,M,JINDEX,F)
C
C       SUBROUTINE FLOWER CALCULATES THE ROTATIONAL ENERGY OF A GIVEN
C       ROTATIONAL STATE(J), VIBRATIONAL STATE(V), AND SPIN STATE(M)
        INTEGER V
        REAL*4 J
        J=JINDEX+.5
        T=0.
        G=0.
        DV=-4.8E-6
        A=124.2
        BE=1.7046
        ALPHAE=.0176
        BV=BE-ALPHAE*(V+.5)
        YV=A/BV
        U=SQRT((J+.5)**2-YV*(1.-YV/4.))
        GO TO(1,2),M
  1     FN=BV*((J+.5)**2-1.-U)+DV*J**4
        GO TO 3
  2     FN=BV*((J+.5)**2-1+U)+DV*(J+1.)**4
  3     F=T+G+FN
        RETURN
        END
```

```
      SUBROUTINE HONNUM(NUP,NUPP,MEGAN,MLGAM,JF,JPP,IB,HONL)
C     SUBROUTINE HONNUM CALCULATES THE HONL-LONDON FACTOR WHERE
C     NUP=UPPER VIBRATIONAL STATE
C     NUPP=LOWER VIBRATIONAL STATE
C     MEGAN=UPPER SPIN STATE
C     MEGAM=LOWER SPIN STATE
C     J=J**
C     IB=1 FOR P BRANCH, =2 FOR Q BRANCH, =3 FOR R BRANCH
C
      REAL*4 J
      J=JPP+.5
      T1=2.*J+1.
      T2=T1*T1
      T3=1./SQRT(73.3*69.3+T2)
      JB=IB+1
      GO TO(2,2,3,4),JB
   2  CONTINUE
      GO TO(21,22),MEGAN
  21  CONTINUE
      GO TO(211,212),MEGAM
 211  RNUM=T2+T1*T3*(4.*J*J+4.*J+1.-146.5)
      DENOM=8.*J
      GO TO 11111
 212  RNUM=T2-T1*T3*(4.*J*J+4.*J+1.-146.5)
      DENOM=8.*J
      GO TO 11111
  22  CONTINUE
      GO TO(221,222),MEGAM
 221  RNUM=T2-T1*T3*(4.*J*J+4.*J-7.+146.5)
      DENOM=8.*J
      GO TO 11111
 222  RNUM=T2+T1*T3*(4.*J*J+4.*J-7+146.5)
      DENOM=8.*J
      GO TO 11111
   3  CONTINUE
      GO TO(31,32),MEGAN
  31  CONTINUE
      GO TO(311,312),MEGAM
 311  RNUM=T1*((4*J*J-4*J-1)+T3*(8.*J**3+12.*J*J-2.*J-7.+146.5))
      DENOM=8.*J*(J+1.)
      GO TO 11111
 312  RNUM=T1*(4.*J*J+4.*J-1.-T3*(8.*J**3+12.*J**2-2.*J-7.+146.5))
      DENOM=8.*J*(J+1.)
      GO TO 11111
  32  CONTINUE
      GO TO(321,322),MEGAM
 321  RNUM=T1*((4.*J*J+4.*J-1.)-T3*(8.*J**3+12.*J*J-2.*J+1.-146.5))
      DENOM=8.*J*(J+1.)
      GO TO 11111
 322  RNUM=T1*((4.*J*J+4.*J-1.)+T3*(8.*J**3+12.*J*J-2.*J+1.-146.5))
      DENOM=8.*J*(J+1.)
      GO TO 11111
   4  CONTINUE
      GO TO(41,42),MEGAN
  41  CONTINUE
      GO TO(411,412),MEGAM
```

```
 411 RNUM=T2+T1*T3*(4.*J*J+4.*J-7.+146.5)
     DENUM=2.*(J+1.)
     GO TO 11111
 412 RNUM=T2-T1*T3*(4.*J*J+4.*J-7.+146.5)
     DENUM=2.*(J+1)
     GO TO 11111
  42 CONTINUE
     GO TO(421,422),PEGAM
 421 RNUM=T2-T1*T3*(4.*J*J+4.*J+1.-146.5)
     DENUM=2.*(J+1.)
     GO TO 11111
 422 RNUM=T2+T1*T3*(4.*J*J+4.*J+1.-146.5)
     DENUM=2.*(J+1.)
11111 CONTINUE
     IF(DENUM.EQ.0)GO TO 591
     HORL=RNUM/DENUM
     RETURN
 591 HORL=0.
     RETURN
     END
```

```
      SUBROUTINE WFUNC(XF,YF,W1,W2)                         W(Z)   1
C
C     XF,YF ARE THE REAL AND IMAGINARY PARTS OF THE ARGUMENT
C     W1,W2 ARE THE REAL AND IMAGINARY PARTS OF THE FUNCTION
C     W(Z)=EXP(-Z**2)ERFC(-IZ)   (SEE NATIONAL BUREAU OF STANDARDS
C     HANDBOOK OF MATHEMATICAL FUNCTIONS, PAGE 297)
C
      IMPLICIT REAL*8(A-H,O-Z)                              W(Z)   2
      COMPLEX*16 ZC,WC,J,ZS,T1,T2,T3                        W(Z)   3
      COMMON/TABLE/Z(31,40,2),X(40),Y(31)                   W(Z)   4
      DIMENSION W(2)                                        W(Z)   5
      IFLAG=0                                               W(Z)   6
      IF(XF.LT.0.)IFLAG=IFLAG+1                             W(Z)   7
      IF(YF.LT.0.)IFLAG=IFLAG+3                             W(Z)   8
      XI=DABS(XF)                                           W(Z)   9
      YI=DABS(YF)                                           W(Z)  10
      IF(XI.GE.3.900.OR.YI.GE.3.D0)GO TO 1                  W(Z)  11
      II=10*YI+1                                            W(Z)  12
      JJ=10*XI+1                                            W(Z)  13
      II1=II+1                                              W(Z)  14
      JJ1=JJ+1                                              W(Z)  15
      DO 10 K=1,2                                           W(Z)  16
      Z1=(Z(II,JJ,K)-Z(II,JJ1,K))*(XI-X(JJ1))/(X(JJ)-X(JJ1))+Z(II,JJ1,K) W(Z) 17
      Z2=(Z(II1,JJ,K)-Z(II1,JJ1,K))*(XI-X(JJ1))/(X(JJ)-X(JJ1))  W(Z)  18
     **+Z(II1,JJ1,K)                                       W(Z)  19
   10 W(K)=(Z1-Z2)*(YI-Y(II1))/(Y(II)-Y(II1))+Z2           W(Z)  20
      W1=W(1)                                               W(Z)  21
      W2=W(2)                                               W(Z)  22
      IF(IFLAG.EQ.0)RETURN                                 W(Z)  23
      GO TO(100,300,300,400),IFLAG                          W(Z)  24
      RETURN                                               W(Z)  25
    1 IF(XI.GT.6.0D0.OR.YI.GT.6.0D0)GO TO 2                W(Z)  26
      J=(0.0D0,1.0D0)                                       W(Z)  27
      ZC=DCMPLX(XI,YI)                                      W(Z)  28
      ZS=ZC*ZC                                              W(Z)  29
      T1=.4613135D0/(ZS-.1901635D0)                         W(Z)  30
      T2=.0999216D0/(ZS-1.7844927D0)                        W(Z)  31
      T3=.0028838D0/(ZS-5.5253437D0)                        W(Z)  32
      WC=J*ZC*(T1+T2+T3)                                    W(Z)  33
      W1=(WC+DCONJG(WC))*.5D0                               W(Z)  34
      W2=(DCONJG(WC)-WC)*J*.5D0                             W(Z)  35
      IF(IFLAG.EQ.0)RETURN                                 W(Z)  36
      GO TO(100,300,300,400),IFLAG                          W(Z)  37
    2 J=(0.0D0,1.0D0)                                       W(Z)  38
      ZC=DCMPLX(XI,YI)                                      W(Z)  39
      ZS=ZC*ZC                                              W(Z)  40
      T1=.5124242D0/(ZS-.2752551D0)                         W(Z)  41
      T2=.0517653D0/(ZS-2.7247446D0)                        W(Z)  42
      WC=J*ZC*(T1+T2)                                       W(Z)  43
      W1=(WC+DCONJG(WC))*.5D0                               W(Z)  44
      W2=(DCONJG(WC)-WC)*J*.5D0                             W(Z)  45
      IF(IFLAG.EQ.0)RETURN                                 W(Z)  46
      GO TO(100,300,300,400),IFLAG                          W(Z)  47
  100 W2=-W2                                                W(Z)  48
      RETURN                                               W(Z)  49
  300 G=2.0D0*DEXP(YI*YI-XI*XI)                             W(Z)  50
```

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```
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        GG=2.D0*XI*YI                                                   W(Z)   51
        #1=G*DCOS(GG)-#1                                                W(Z)   52
        #2=G*DSIN(GG)+#2                                                #(Z)   53
        RETURN                                                          W(Z)   54
    406 G=2.D0*DEXP(YI*YI-XI*XI)                                        W(Z)   55
        GG=2.D0*XI*YI                                                   #(Z)   56
        #1=G*DCOS(GG)-#1                                                W(Z)   57
        #2=-G*DSIN(GG)-#2                                               W(Z)   58
        RETURN                                                          W(Z)   59
        END                                                            #(Z)   60
```

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```
      BLOCK DATA                                                    W(Z)  61
      IMPLICIT REAL*8(A-H,O-Z)                                      W(Z)  62
      COMMON/TABLE/                                                 W(Z)  63
     *Z 1(31),   Z 2(31),   Z 3(31),   Z 4(31),   Z 5(31),   Z 6(31),Z 7(31),W(Z)  64
     *Z 8(31),   Z 9(31),   Z10(31),   Z11(31),   Z12(31),   Z13(31),Z14(31),W(Z)  65
     *Z15(31),   Z16(31),   Z17(31),   Z18(31),   Z19(31),   Z20(31),Z21(31),W(Z)  66
     *Z22(31),   Z23(31),   Z24(31),   Z25(31),   Z26(31),   Z27(31),Z28(31),W(Z)  67
     *Z29(31),   Z30(31),   Z31(31),   Z32(31),   Z33(31),   Z34(31),Z35(31),W(Z)  68
     *Z36(31),   Z37(31),   Z38(31),   Z39(31),   Z40(31),   Z41(31),Z42(31),W(Z)  69
     *Z43(31),   Z44(31),   Z45(31),   Z46(31),   Z47(31),   Z48(31),Z49(31),W(Z)  70
     *Z50(31),   Z51(31),   Z52(31),   Z53(31),   Z54(31),   Z55(31),Z56(31),W(Z)  71
     *Z57(31),   Z58(31),   Z59(31),   Z60(31),   Z61(31),   Z62(31),Z63(31),W(Z)  72
     *Z64(31),   Z65(31),   Z66(31),   Z67(31),   Z68(31),   Z69(11),Z70(31),W(Z)  73
     *Z71(31),   Z72(31),   Z73(31),   Z74(31),   Z75(31),   Z76(31),Z77(31),W(Z)  74
     *Z78(31),   Z79(31),   Z80(31),                                W(Z)  75
     *X(40),Y(31)                                                   W(Z)  76
      DATA X/0.00,.100,.200,.300,.400,.500,.600,.700,.800,.900,     W(Z)  77
     *1.000,1.100,1.200,1.300,1.400,1.500,1.600,1.700,1.800,1.900,  W(Z)  78
     *2.000,2.100,2.200,2.300,2.400,2.500,2.600,2.700,2.800,2.900,  W(Z)  79
     *3.000,3.100,3.200,3.300,3.400,3.500,3.600,3.700,3.800,3.900/  W(Z)  80
      DATA Y/0.00,.100,.200,.300,.400,.500,.600,.700,.800,.900,1.000,W(Z)  81
     *1.100,1.200,1.300,1.400,1.500,1.600,1.700,1.800,1.900,2.000,  W(Z)  82
     *2.100,2.200,2.300,2.400,2.500,2.600,2.700,2.800,2.900,3.000/  W(Z)  83
      DATA Z 1/                                                      W(Z)  84
     *1.0000000,    .69845700,    .50902000,    .73459900,    .67078800,  W(Z)  85
     *  .61964900,   .56780500,   .52593000,   .45910100,   .45605200,   W(Z)  86
     *  .42726400,   .40173000,   .37653700,   .35764300,   .33874400,   W(Z)  87
     *  .32155500,   .30555300,   .25100500,   .27850000,   .26650900,   W(Z)  88
     *  .25235600,   .24511900,   .23559300,   .22674200,   .21849900,   W(Z)  89
     *  .21020000,   .20301300,   .15667400,   .19054900,   .18460200,   W(Z)  90
     *  .17900100/                                                        W(Z)  91
      DATA Z 2/                                                           W(Z)  92
     *  .59002000,   .80847500,   .60236700,   .72933700,   .66646300,   W(Z)  93
     *  .61210500,   .56461800,   .52342300,   .48698200,   .45473100,   W(Z)  94
     *  .42604400,   .40064000,   .37739300,   .35664900,   .33787600,   W(Z)  95
     *  .32062500,   .30624400,   .25107200,   .27803500,   .26604200,   W(Z)  96
     *  .25467200,   .24474500,   .23525600,   .22643800,   .21822400,   W(Z)  97
     *  .21055700,   .20338700,   .16006600,   .19036000,   .18442900,   W(Z)  98
     *  .17864200/                                                        W(Z)  99
      DATA Z 3/                                                           W(Z) 100
     *  .90076500,   .82449800,   .76353800,   .71390100,   .65368000,   W(Z) 101
     *  .60131300,   .55957400,   .51599100,   .48069700,   .44938300,   W(Z) 102
     *  .42148800,   .34647000,   .37396900,   .35369100,   .33529400,   W(Z) 103
     *  .31850100,   .33329000,   .28930900,   .27647000,   .26464800,   W(Z) 104
     *  .25372200,   .24362800,   .23425100,   .22553100,   .21740400,   W(Z) 105
     *  .20961300,   .20271000,   .19605000,   .18979600,   .18391200,   W(Z) 106
     *  .17834200/                                                        W(Z) 107
      DATA Z 4/                                                           W(Z) 108
     *  .51393100,   .82724800,   .75289500,   .68872000,   .63299800,   W(Z) 109
     *  .58493300,   .54160500,   .50309600,   .47045200,   .44065000,   W(Z) 110
     *  .41359400,   .35602800,   .30641200,   .34883900,   .33105400,   W(Z) 111
     *  .31463500,   .30000900,   .28640800,   .27389200,   .26235000,   W(Z) 112
     *  .25167700,   .24178300,   .23259200,   .22493300,   .21604700,   W(Z) 113
     *  .20852200,   .20152900,   .19502800,   .18886100,   .18309600,   W(Z) 114
     *  .17758100/                                                        W(Z) 115
      DATA Z 5/                                                           W(Z) 116
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IV G LEVEL  21              BLK DATA         DATE = 75178         09/06/45

     *  .8321440O,   .7772670O,   .7121460O,   .6552440O,   .6052950O,   W(Z) 117
     *  .5612520O,   .5222460C,   .4875560O,   .4565790O,   .4288080O,   W(Z) 118
     *  .4038180O,   .3812500O,   .3607990O,   .3422060O,   .3252480O,   W(Z) 119
     *  .3047360O,   .2955060C,   .2824170O,   .2703460O,   .2591860O,   W(Z) 120
     *  .2488440O,   .2392390C,   .2303000O,   .2219630O,   .2141720O,   W(Z) 121
     *  .2068790O,   .2003900C,   .1930130O,   .1875660O,   .1818680O,   W(Z) 122
     *  .1704510O/                                                        W(Z) 123
        DATA Z 6/                                                         W(Z) 124
     *  .7788010O,   .7175880O,   .6632230O,   .6148520O,   .5717170O,   W(Z) 125
     *  .5331570O,   .4985510C,   .4675210O,   .4395120O,   .4141910O,   W(Z) 126
     *  .3912340O,   .3703630O,   .3513350O,   .3339420O,   .3180010O,   W(Z) 127
     *  .3033250O,   .2896060C,   .2774120O,   .2658900O,   .2552050O,   W(Z) 128
     *  .2452760C,   .2360310C,   .2274070O,   .2193470O,   .2118000O,   W(Z) 129
     *  .2047230O,   .1982740C,   .1918180O,   .1859240O,   .1803610O,   W(Z) 130
     *  .1751050O/                                                        W(Z) 131
        DATA Z 7/                                                         W(Z) 132
     *  .6476760O,   .6516760C,   .6083220O,   .5692380O,   .5335810O,   W(Z) 133
     *  .5010790O,   .4714530O,   .4444340O,   .4197060O,   .3972160O,   W(Z) 134
     *  .3765710C,   .3576370C,   .3402410O,   .3242290O,   .3094630O,   W(Z) 135
     *  .2958200C,   .2831520O,   .2714790O,   .2605980O,   .2504690O,   W(Z) 136
     *  .2410250O,   .2322040O,   .2239520O,   .2162190O,   .2089610O,   W(Z) 137
     *  .2021390O,   .1957170C,   .1896640O,   .1839500O,   .1785490O,   W(Z) 138
     *  .1734370O/                                                        W(Z) 139
        DATA Z 8/                                                         W(Z) 140
     *  .6126260O,   .5806980O,   .5497390O,   .5201920O,   .4922890O,   W(Z) 141
     *  .4660127OC,   .4417120C,   .4189980O,   .3979060O,   .3783410O,   W(Z) 142
     *  .3602000O,   .3433760C,   .3277060O,   .3132730O,   .2998040O,   W(Z) 143
     *  .2872740O,   .2756020C,   .2647180O,   .2545540O,   .2450500O,   W(Z) 144
     *  .2361520O,   .2278100C,   .2199780O,   .2126160O,   .2056860O,   W(Z) 145
     *  .1991550O,   .1929520G,   .1871700O,   .1816620O,   .1764470O,   W(Z) 146
     *  .1715020O/                                                        W(Z) 147
        DATA Z 9/                                                         W(Z) 148
     *  .5272920O,   .5052490O,   .4897100O,   .4694800O,   .4492440O,   W(Z) 149
     *  .4294160O,   .4102640O,   .3919360O,   .3745180O,   .3580430O,   W(Z) 150
     *  .3425110O,   .3275000C,   .3141760O,   .3012940O,   .2892080O,   W(Z) 151
     *  .2778690O,   .2672260O,   .2572370O,   .2478510O,   .2390270O,   W(Z) 152
     *  .2307240C,   .2225050O,   .2155350O,   .2085810O,   .2020130O,   W(Z) 153
     *  .1958040O,   .1895280O,   .1843620O,   .1790840O,   .1740740O,   W(Z) 154
     *  .1693150O/                                                        W(Z) 155
        DATA Z10/                                                         W(Z) 156
     *  .4448580O,   .4394210O,   .4302710O,   .4187360O,   .4057630O,   W(Z) 157
     *  .3920210O,   .3775770O,   .3639570O,   .3501820O,   .3367990O,   W(Z) 158
     *  .3234590O,   .3115370O,   .2994740O,   .2885190O,   .2778650O,   W(Z) 159
     *  .2677060C,   .2582030O,   .2491510O,   .2405800O,   .2324820O,   W(Z) 160
     *  .2246130C,   .2175520C,   .2106700O,   .2041600O,   .1979820O,   W(Z) 161
     *  .1921200O,   .1865540C,   .1812650O,   .1762370O,   .1714520O,   W(Z) 162
     *  .1668950O/                                                        W(Z) 163
        DATA Z11/                                                         W(Z) 164
     *  .3678790O,   .3731710O,   .3731530O,   .3693860O,   .3630200O,   W(Z) 165
     *  .3545060O,   .3456490O,   .3357210O,   .3254460O,   .3150640O,   W(Z) 166
     *  .3047440O,   .2954060O,   .2847310O,   .2751740O,   .2659670O,   W(Z) 167
     *  .2571280O,   .2486650O,   .2405780O,   .2328610O,   .2255030O,   W(Z) 168
     *  .2184930O,   .2118160C,   .2054570O,   .1994020O,   .1936340O,   W(Z) 169
     *  .1881390O,   .1825030O,   .1779100O,   .1731470O,   .1686020O,   W(Z) 170
     *  .1642610O/                                                        W(Z) 171
        DATA Z12/                                                         W(Z) 172
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IV G LEVEL  21              BLK DATA          DATE = 75178              09/06/45

       *  .298157D0,    .312136D0,    .319717D0,    .322586D0,    .32199300,   W(Z) 173
       *  .318884D0,    .313578DC,    .30781600,    .30080700,    .29325900,   W(Z) 174
       *  .285402D0,    .27740700,    .26940100,    .26147600,    .253697D0,   W(Z) 175
       *  .24611200,    .23875200,    .23163500,    .22477500,    .21817600,   W(Z) 176
       *  .21183900,    .20576000,    .19993500,    .19435600,    .18901400,   W(Z) 177
       *  .18359010,    .17900600,    .17432400,    .16984000,    .16554600,   W(Z) 178
       *  .16143400/                                                           W(Z) 179
          DATA Z13/                                                            W(Z) 180
       *  .236628D0,    .25737400,    .27092800,    .27919900,    .28344300,   W(Z) 181
       *  .28402800,    .28354000,    .28074000,    .27669300,    .27175200,   W(Z) 182
       *  .26018600,    .26021300,    .25368500,    .24762800,    .24123300,   W(Z) 183
       *  .23487000,    .22859200,    .22243600,    .21642800,    .21058700,   W(Z) 184
       *  .20492600,    .19945200,    .19416600,    .18907200,    .18416500,   W(Z) 185
       *  .17944400,    .17456300,    .17053800,    .16634200,    .16231000,   W(Z) 186
       *  .15843500/                                                           W(Z) 187
          DATA Z14/                                                            W(Z) 188
      '*  .18452000,    .26943100,    .22736200,    .23979300,    .24790800,   W(Z) 189
       *  .25265400,    .26478400,    .25489500,    .25346100,    .25085800,   W(Z) 190
       *  .24738100,    .24326600,    .23869500,    .23381300,    .22873300,   W(Z) 191
       *  .22354200,    .21830900,    .21308600,    .20791200,    .20281800,   W(Z) 192
       *  .19782700,    .19265300,    .18820600,    .18359900,    .17913100,   W(Z) 193
       *  .17480500,    .17062300,    .16658200,    .16268100,    .15891600,   W(Z) 194
       *  .15528500/                                                           W(Z) 195
          DATA Z15/                                                            W(Z) 196
       *  .14085800,    .16840700,    .18924700,    .20466200,    .21571100,   W(Z) 197
       *  .22326200,    .22812600,    .23057800,    .23138500,    .23082600,   W(Z) 198
       *  .22920500,    .22676700,    .22371000,    .22019200,    .21634000,   W(Z) 199
       *  .21225300,    .20801400,    .20368400,    .19931500,    .19494700,   W(Z) 200
       *  .19066800,    .18632400,    .18211200,    .17798500,    .17395400,   W(Z) 201
       *  .17002400,    .16620100,    .16248700,    .15888300,    .15536900,   W(Z) 202
       *  .15200500/                                                           W(Z) 203
          DATA Z16/                                                            W(Z) 204
       *  .10539900,    .13464900,    .15652100,    .17386500,    .18698400,   W(Z) 205
       *  .19063000,    .20346100,    .20795000,    .21066400,    .21184600,   W(Z) 206
       *  .21182700,    .21088100,    .20918200,    .20690200,    .20417700,   W(Z) 207
       *  .20111500,    .14786600,    .19432000,    .19071700,    .18704300,   W(Z) 208
       *  .18353500,    .17982300,    .17593000,    .17227600,    .16867400,   W(Z) 209
       *  .16512600,    .16166500,    .15828100,    .15497500,    .15175300,   W(Z) 210
       *  .14801800/                                                           W(Z) 211
          DATA Z17/                                                            W(Z) 212
       *  .07730500,    .10584300,    .12889500,    .14727200,    .16170200,   W(Z) 213
       *  .17282000,    .18117700,    .18724500,    .19142300,    .19404900,   W(Z) 214
       *  .19540700,    .19573400,    .19522800,    .19405300,    .19234700,   W(Z) 215
       *  .19022200,    .18777200,    .18507300,    .18218900,    .17917200,   W(Z) 216
       *  .17600400,    .17290100,    .16971000,    .16651300,    .16333000,   W(Z) 217
       *  .16017500,    .15706600,    .15399300,    .15098100,    .14803000,   W(Z) 218
       *  .14514400/                                                           W(Z) 219
          DATA Z18/                                                            W(Z) 220
       *  .05567000,    .08311200,    .10592900,    .12461200,    .13971700,   W(Z) 221
       *  .15175100,    .16117100,    .16837900,    .17372500,    .17751300,   W(Z) 222
       *  .18000200,    .18141400,    .18193800,    .18173300,    .18093300,   W(Z) 223
       *  .17965100,    .17798300,    .17600800,    .17379200,    .17139000,   W(Z) 224
       *  .16884900,    .16620600,    .16349300,    .16073700,    .15795800,   W(Z) 225
       *  .15517600,    .15240200,    .14964900,    .14692700,    .14424300,   W(Z) 226
       *  .14160200/                                                           W(Z) 227
          DATA Z19/                                                            W(Z) 228
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IV G LEVEL   21              BLK DATA           DATE = 75178          09/06/45

      *  .C3910400,  .0e5C99D0,  .04709000,  .10662200,  .12079300,   W(Z) 229
      *  .1332e600,  .143369DJ,  .131366DJ,  .15757600,  .16226600,   W(Z) 230
      *  .1656e7DJ,  .16757700,  .16937300,  .17000300,  .16939700,   W(Z) 231
      *  .16946600,  .1685C0D0,  .16718300,  .16537900,  .16374600,   W(Z) 232
      *  .1617c3DJ,  .1595e0DC,  .15732000,  .15494200,  .15259100,   W(Z) 233
      *  .15016600,  .14772200,  .14527400,  .14283400,  .14041100,   W(Z) 234
      *  .13ec120J/                                                   W(Z) 235
         DATA Z20/                                                    W(Z) 236
      *  .027692DJ,  .C51C3800,  .07181100,  .08959200,  .10404100,   W(Z) 237
      *  .1172330J,  .12764400,  .13013400,  .14294900,  .14631000,   W(Z) 238
      *  .15241800,  .15649200,  .15756900,  .15890600,  .15958500,   W(Z) 239
      *  .15970900,  .13536900,  .15864100,  .15759300,  .15628200,   W(Z) 240
      *  .15475700,  .15365900,  .15122400,  .14928100,  .14725600,   W(Z) 241
      *  .14517200,  .14304500,  .14089200,  .13872500,  .13655500,   W(Z) 242
      *  .13435100/                                                   W(Z) 243
         DATA Z21/                                                    W(Z) 244
      *  .01831600,  .0492c0100,  .05953100,  .07639600,  .09094400,   W(Z) 245
      *  .10335400,  .11363c00,  .12257400,  .12970600,  .13560000,   W(Z) 246
      *  .14024000,  .14364400,  .14664100,  .14646600,  .14972500,   W(Z) 247
      *  .15041500,  .15062200,  .15041600,  .14987000,  .14903200,   W(Z) 248
      *  .14795300,  .14667500,  .14523400,  .14366000,  .14196200,   W(Z) 249
      *  .14022000,  .13835500,  .13652300,  .13461900,  .13269300,   W(Z) 250
      *  .13072700/                                                   W(Z) 251
         DATA Z22/                                                    W(Z) 252
      *  .01213500,  .03153600,  .04972600,  .06552100,  .07936500,   W(Z) 253
      *  .09142200,  .10176500,  .11055400,  .11794400,  .12408100,   W(Z) 254
      *  .12909700,  .13312500,  .13026e00,  .13860900,  .14043200,   W(Z) 255
      *  .14166400,  .14228500,  .14254300,  .14243400,  .14202100,   W(Z) 256
      *  .14134700,  .14046300,  .13937500,  .13614500,  .13678900,   W(Z) 257
      *  .13533100,  .13379100,  .13218700,  .13053300,  .12884200,   W(Z) 258
      *  .12712500/                                                   W(Z) 259
         DATA Z23/                                                    W(Z) 260
      *  .00796700,  .025e7800,  .04192700,  .05656600,  .06965500,   W(Z) 261
      *  .08116200,  .09124500,  .09994300,  .10738300,  .11367900,   W(Z) 262
      *  .11694100,  .12327700,  .12676600,  .12957000,  .13170900,   W(Z) 263
      *  .13326400,  .13436700,  .13502100,  .13534500,  .13526900,   W(Z) 264
      *  .13495500,  .13441400,  .13366900,  .13275500,  .13169900,   W(Z) 265
      *  .13052400,  .12925200,  .12790000,  .12646300,  .12501600,   W(Z) 266
      *  .12351000/                                                   W(Z) 267
         DATA Z24/                                                    W(Z) 268
      *  .00564200,  .02065500,  .03572300,  .04924600,  .06147300,   W(Z) 269
      *  .07240300,  .08214200,  .09058300,  .09796300,  .10430900,   W(Z) 270
      *  .10976900,  .11425100,  .11861900,  .12109200,  .12354600,   W(Z) 271
      *  .12543400,  .12667700,  .12767300,  .12849500,  .12879200,   W(Z) 272
      *  .12880500,  .12857400,  .12813000,  .12750600,  .12672600,   W(Z) 273
      *  .12581400,  .12475200,  .12367000,  .12248400,  .12122900,   W(Z) 274
      *  .11942200/                                                   W(Z) 275
         DATA Z25/                                                    W(Z) 276
      *  .00315100,  .01735700,  .03079200,  .04321100,  .05458500,   W(Z) 277
      *  .06469300,  .07419200,  .08234500,  .08957600,  .09588400,   W(Z) 278
      *  .10133600,  .10599900,  .10994200,  .11323200,  .11593500,   W(Z) 279
      *  .11816900,  .11982000,  .12109600,  .12201000,  .12259700,   W(Z) 280
      *  .12285700,  .12294500,  .12277300,  .12241100,  .12184400,   W(Z) 281
      *  .12121500,  .12042400,  .11953300,  .11854800,  .11749200,   W(Z) 282
      *  .11637500/                                                   W(Z) 283
         DATA Z26/                                                    W(Z) 284
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    *  .00193000,    .01465800,    .02684100,    .03822600,    .04877300,    W(Z) 285
    *  .05843700,    .06720500,    .07508800,    .08211200,    .08831700,    W(Z) 286
    *  .09375100,    .05846600,    .10251800,    .10596000,    .10884800,    W(Z) 287
    *  .11123300,    .11316500,    .11469000,    .11585100,    .11668900,    W(Z) 288
    *  .11723900,    .11753400,    .11760000,    .11748100,    .11718400,    W(Z) 289
    *  .11673700,    .11616000,    .115471D0,    .11468500,    .11381600,    W(Z) 290
    *  .11267800/                                                            W(Z) 291
       DATA Z27/                                                             W(Z) 292
    *  .00115900,    .01263500,    .02365300,    .03408700,    .04384900,    W(Z) 293
    *  .05288500,    .06116700,    .06869100,    .07546700,    .08152100,    W(Z) 294
    *  .08686500,    .09155800,    .09570200,    .09924300,    .10226400,    W(Z) 295
    *  .10481100,    .10652500,    .10864700,    .11001600,    .11106700,    W(Z) 296
    *  .11183400,    .11234700,    .11263500,    .11272300,    .11263300,    W(Z) 297
    *  .11238900,    .11200800,    .11150800,    .11090400,    .11021000,    W(Z) 298
    *  .10943900/                                                            W(Z) 299
       DATA Z28/                                                             W(Z) 300
    *  .00068200,    .01103700,    .02105700,    .03062600,    .03965600,    W(Z) 301
    *  .04809000,    .05589000,    .06304300,    .06954800,    .07541600,    W(Z) 302
    *  .08067000,    .08533800,    .08945100,    .09304400,    .09615500,    W(Z) 303
    *  .09882000,    .10107600,    .10295700,    .10449800,    .10573000,    W(Z) 304
    *  .10668300,    .10738600,    .10786400,    .10814000,    .10823800,    W(Z) 305
    *  .10817700,    .10797500,    .10764800,    .10721300,    .10668200,    W(Z) 306
    *  .10606700/                                                            W(Z) 307
       DATA Z29/                                                             W(Z) 308
    *  .00039400,    .00977800,    .01891800,    .02770700,    .03606400,    W(Z) 309
    *  .04393000,    .05126400,    .05804600,    .06426600,    .06992700,    W(Z) 310
    *  .07504300,    .07963200,    .08371600,    .08732800,    .09049200,    W(Z) 311
    *  .09323900,    .09560100,    .09760800,    .09928800,    .10067100,    W(Z) 312
    *  .10178300,    .10264900,    .10329300,    .10373700,    .10400200,    W(Z) 313
    *  .10410500,    .10406600,    .10389800,    .10361700,    .10323600,    W(Z) 314
    *  .10276700/                                                            W(Z) 315
       DATA Z30/                                                             W(Z) 316
    *  .00022300,    .00876900,    .01771300,    .02522500,    .03296700,    W(Z) 317
    *  .04030400,    .04719400,    .05361100,    .05954300,    .06498600,    W(Z) 318
    *  .06994400,    .07443100,    .07846200,    .08205900,    .08524500,    W(Z) 319
    *  .08804400,    .09048200,    .09258400,    .09437600,    .09588200,    W(Z) 320
    *  .09712700,    .09813300,    .09892200,    .09951300,    .09992500,    W(Z) 321
    *  .10017700,    .10028400,    .10026100,    .10012200,    .09987900,    W(Z) 322
    *  .09954400/                                                            W(Z) 323
       DATA Z31/                                                             W(Z) 324
    *  .00012300,    .00754300,    .01562700,    .02309500,    .03027900,    W(Z) 325
    *  .03712600,    .04359800,    .04966500,    .05531100,    .06052900,    W(Z) 326
    *  .06531800,    .06968500,    .07364100,    .07720200,    .08038500,    W(Z) 327
    *  .08321000,    .08565700,    .08787000,    .08974900,    .09135500,    W(Z) 328
    *  .09271100,    .09383500,    .09474800,    .09546700,    .09601000,    W(Z) 329
    *  .09639300,    .09663200,    .09673900,    .09672900,    .09661300,    W(Z) 330
    *  .09640200/                                                            W(Z) 331
       DATA Z32/                                                             W(Z) 332
    *  .00006700,    .00725400,    .01433800,    .02125000,    .02792900,    W(Z) 333
    *  .03432800,    .04040700,    .04614100,    .05150900,    .05650100,    W(Z) 334
    *  .06111400,    .06535000,    .06921600,    .07272200,    .07588300,    W(Z) 335
    *  .07871200,    .08122900,    .08345000,    .08539400,    .08708000,    W(Z) 336
    *  .08852500,    .08974900,    .09076700,    .09159700,    .09225500,    W(Z) 337
    *  .09275400,    .09311000,    .09333600,    .09344200,    .09344200,    W(Z) 338
    *  .09334500/                                                            W(Z) 339
       DATA Z33/                                                             W(Z) 340
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IV C LEVEL   21   BLK DATA   DATE = 75178   09/06/45

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    * .00003600,  .00667000,  .01322500,  .01963900,  .02586200,   W(Z) 341
    * .03184900,  .03756500,  .04298300,  .04806300,  .05285400,   W(Z) 342
    * .05722400,  .06138700,  .06515100,  .06858900,  .07171100,   W(Z) 343
    * .07452900,  .07725500,  .07930600,  .08129700,  .08304400,   W(Z) 344
    * .08464200,  .08586700,  .08697400,  .08790000,  .08865700,   W(Z) 345
    * .08922900,  .08971900,  .09005000,  .09026300,  .09036800,   W(Z) 346
    * .09037500/                                                    W(Z) 347
      DATA Z34/                                                     W(Z) 348
    * .00001900,  .00616700,  .01225200,  .01822200,  .02403200,   W(Z) 349
    * .02964300,  .03502200,  .04014400,  .04498900,  .04954400,   W(Z) 350
    * .05380100,  .05775700,  .06141300,  .06477300,  .06784400,   W(Z) 351
    * .07063600,  .07315600,  .07542300,  .07744500,  .07923600,   W(Z) 352
    * .08081100,  .08218200,  .08336400,  .08437000,  .08521300,   W(Z) 353
    * .08590500,  .08645200,  .08688300,  .08719000,  .08739100,   W(Z) 354
    * .08749300/                                                    W(Z) 355
      DATA Z35/                                                     W(Z) 356
    * .00001000,  .00572800,  .01139400,  .01696600,  .02240300,   W(Z) 357
    * .02767000,  .03273800,  .03758200,  .04218500,  .04653200,   W(Z) 358
    * .05061500,  .05442600,  .05797100,  .06124000,  .06425800,   W(Z) 359
    * .06701200,  .06951600,  .07178500,  .07362300,  .07564600,   W(Z) 360
    * .07724300,  .07868700,  .07995000,  .08100400,  .08192100,   W(Z) 361
    * .08224900,  .08332400,  .08383200,  .08422500,  .08451100,   W(Z) 362
    * .08474000/                                                    W(Z) 363
      DATA Z36/                                                     W(Z) 364
    * .00000300,  .00534000,  .01063300,  .01584600,  .02094400,   W(Z) 365
    * .02505700,  .03062700,  .03526300,  .03963700,  .04378500,   W(Z) 366
    * .04765200,  .05137000,  .05479800,  .05798400,  .06092800,   W(Z) 367
    * .06303700,  .06611600,  .06837400,  .07041900,  .07226000,   W(Z) 368
    * .07395600,  .07537300,  .07666600,  .07779600,  .07877400,   W(Z) 369
    * .07961100,  .08031600,  .08089800,  .08136600,  .08173000,   W(Z) 370
    * .08159600/                                                    W(Z) 371
      DATA Z37/                                                     W(Z) 372
    * .00000200,  .00495500,  .00995200,  .01484100,  .01963200,   W(Z) 373
    * .02424700,  .02861200,  .03315800,  .03731600,  .04127400,   W(Z) 374
    * .04502300,  .04855000,  .05186900,  .05496200,  .05783500,   W(Z) 375
    * .06064100,  .06243600,  .06517600,  .06721700,  .06906800,   W(Z) 376
    * .07072600,  .07223200,  .07356300,  .07473900,  .07577000,   W(Z) 377
    * .07664400,  .07743600,  .07807600,  .07861200,  .07904400,   W(Z) 378
    * .07920100/                                                    W(Z) 379
      DATA Z38/                                                     W(Z) 380
    * .00000100,  .00468500,  .00933900,  .01393500,  .01844600,   W(Z) 381
    * .02264700,  .02711800,  .03123900,  .03519500,  .03897400,   W(Z) 382
    * .04255200,  .04556200,  .04916100,  .05215900,  .05495800,   W(Z) 383
    * .05755700,  .05955200,  .06217700,  .06420600,  .06605800,   W(Z) 384
    * .06773800,  .06925400,  .07061500,  .07182900,  .07290200,   W(Z) 385
    * .07304500,  .07460300,  .07536600,  .07596100,  .07645500,   W(Z) 386
    * .07685500/                                                    W(Z) 387
      DATA Z39/                                                     W(Z) 388
    * .00000100,  .00440600,  .00878600,  .01311500,  .01737000,   W(Z) 389
    * .02152900,  .02557400,  .02946000,  .03325300,  .03686100,   W(Z) 390
    * .04036100,  .04352700,  .04665300,  .04955800,  .05227900,   W(Z) 391
    * .05431900,  .05717900,  .05936200,  .06137400,  .06321900,   W(Z) 392
    * .06490300,  .06643300,  .06781500,  .06905800,  .07016600,   W(Z) 393
    * .07114400,  .07261300,  .07276400,  .07341100,  .07395900,   W(Z) 394
    * .07441900/                                                    W(Z) 395
      DATA Z40/                                                     W(Z) 396
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IV G LEVEL  21              BLK DATA          DATE = 75178           09/06/45

   *  .00300003,   .00415300,   .00828200,   .01236800,   .01638900,   W(Z) 397
   *  .02003000,   .02416200,   .02768000,   .03146900,   .03491600,   W(Z) 398
   *  .03821200,   .04135200,   .04432800,   .04713900,   .04978300,   W(Z) 399
   *  .05222003,   .05457200,   .05672000,   .05870800,   .06054000,   W(Z) 400
   *  .06222200,   .06375900,   .06515800,   .06642000,   .06755600,   W(Z) 401
   *  .06857200,   .06947400,   .07026700,   .07095900,   .07155500,   W(Z) 402
   +  .07206100/                                                        W(Z) 403
      DATA Z41/                                                         W(Z) 404
   *  .00000000,   .00000000,   .00000000,   .00000000,   .00000000,   W(Z) 405
   *  .00000000,   .00000000,   .00000000,   .00000000,   .00000000,   W(Z) 406
   *  .00000000,   .00000000,   .00000000,   .00000000,   .00000000,   W(Z) 407
   *  .00000000,   .00000000,   .00000000,   .00000000,   .00000000,   W(Z) 408
   *  .00000000,   .00000000,   .00000000,   .00000000,   .00000000,   W(Z) 409
   *  .00000000,   .00000000,   .00000000,   .00000000,   .00000000,   W(Z) 410
   +  .00000000/                                                        W(Z) 411
      DATA Z42/                                                         W(Z) 412
   *  .11200900,   .05433200,   .00002900,   .06841000,   .05889700,   W(Z) 413
   *  .05104300,   .04452400,   .03906400,   .03440500,   .03056600,   W(Z) 414
   *  .02724200,   .02433200,   .02153400,   .01980500,   .01795100,   W(Z) 415
   *  .01032900,   .01490500,   .01364300,   .01253600,   .01154700,   W(Z) 416
   *  .01066400,   .00987400,   .00910300,   .00852600,   .00794900,   W(Z) 417
   *  .00742700,   .00695200,   .00652200,   .00612500,   .00576400,   W(Z) 418
   +  .00543300/                                                        W(Z) 419
      DATA Z43/                                                         W(Z) 420
   *  .21973900,   .16222200,   .15740300,   .13473900,   .11614700,   W(Z) 421
   *  .10070200,   .08799300,   .07727500,   .06823500,   .06056300,   W(Z) 422
   *  .05341400,   .04833500,   .04354200,   .03933600,   .03567100,   W(Z) 423
   *  .03242300,   .02904300,   .02713400,   .02494800,   .02298700,   W(Z) 424
   *  .02123200,   .01922900,   .01826000,   .01679100,   .01584500,   W(Z) 425
   *  .01480000,   .01382200,   .01300200,   .01221600,   .01149800,   W(Z) 426
   +  .01063300/                                                        W(Z) 427
      DATA Z44/                                                         W(Z) 428
   *  .31091600,   .26906900,   .22905300,   .19703700,   .17020300,   W(Z) 429
   *  .14755200,   .12944600,   .11382100,   .10004700,   .08944400,   W(Z) 430
   *  .07906400,   .07162200,   .06451000,   .05832900,   .05293600,   W(Z) 431
   *  .04802100,   .04465100,   .04037700,   .03711800,   .03421700,   W(Z) 432
   *  .03102600,   .02931400,   .02721700,   .02533500,   .02363300,   W(Z) 433
   *  .02225900,   .02062700,   .01940900,   .01824100,   .01717200,   W(Z) 434
   +  .01615200/                                                        W(Z) 435
      DATA Z45/                                                         W(Z) 436
   *  .40615300,   .34406800,   .29405300,   .25361300,   .21970600,   W(Z) 437
   *  .19150000,   .16708600,   .14757500,   .13110100,   .11671400,   W(Z) 438
   *  .10428000,   .09375200,   .08434700,   .07653800,   .06903800,   W(Z) 439
   *  .06353900,   .05757600,   .05316800,   .04873100,   .04511900,   W(Z) 440
   *  .04174800,   .03876000,   .03596800,   .03349600,   .03120300,   W(Z) 441
   *  .02922400,   .02736900,   .02570000,   .02416800,   .02275900,   W(Z) 442
   +  .02146000/                                                        W(Z) 443
      DATA Z46/                                                         W(Z) 444
   *  .47092500,   .40047400,   .35075100,   .30312400,   .26350300,   W(Z) 445
   *  .23048800,   .20260000,   .17912300,   .15906700,   .14194500,   W(Z) 446
   *  .12720200,   .11446000,   .10334500,   .09374400,   .08528000,   W(Z) 447
   *  .07782100,   .07122300,   .06540100,   .06026300,   .05560100,   W(Z) 448
   *  .05152100,   .04780400,   .04445400,   .04142300,   .03868000,   W(Z) 449
   *  .03619600,   .03392500,   .03185900,   .02996000,   .02823100,   W(Z) 450
   +  .02603000/                                                        W(Z) 451
      DATA Z47/                                                         W(Z) 452
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IV G LEVEL  21              BLK DATA        DATE = 75178        09/06/45

      *  .53571300,  .45966500,  .39685200,  .34464500,  .30098900,      W(Z)  453
      *  .26426800,  .23320690,  .20678700,  .18420000,  .16479300,      W(Z)  454
      *  .14803600,  .13356100,  .12083800,  .10975900,  .10002600,      W(Z)  455
      *  .09144300,  .08384500,  .07709600,  .07108100,  .06570100,      W(Z)  456
      *  .06087600,  .05653400,  .05261700,  .04907300,  .04585900,      W(Z)  457
      *  .04293600,  .04027100,  .03783600,  .03560700,  .03356100,      W(Z)  458
      *  .03168000/                                                      W(Z)  459
         DATA Z48/                                                       W(Z)  460
      *  .57604200,  .45774400,  .43244200,  .37766800,  .33153500,      W(Z)  461
      *  .29243200,  .25913600,  .23064600,  .20615500,  .18500500,      W(Z)  462
      *  .16662000,  .15066100,  .13670600,  .12443500,  .11362000,      W(Z)  463
      *  .10405400,  .09556300,  .08800100,  .08124500,  .07519000,      W(Z)  464
      *  .06974800,  .06484200,  .06040900,  .05639100,  .05274100,      W(Z)  465
      *  .04941700,  .04636400,  .04360800,  .04106400,  .03872800,      W(Z)  466
      *  .03657700/                                                      W(Z)  467
         DATA Z49/                                                       W(Z)  468
      *  .60041200,  .52293200,  .45756900,  .40219400,  .35508200,      W(Z)  469
      *  .31482800,  .28029000,  .25053200,  .22478900,  .20242900,      W(Z)  470
      *  .18293200,  .16586800,  .15087700,  .13766100,  .12597100,      W(Z)  471
      *  .11565400,  .10635500,  .09810300,  .09071000,  .08406800,      W(Z)  472
      *  .07808500,  .07266000,  .06778500,  .06334200,  .05929800,      W(Z)  473
      *  .05561600,  .05223600,  .04915600,  .04631500,  .04370800,      W(Z)  474
      *  .04130600/                                                      W(Z)  475
         DATA Z50/                                                       W(Z)  476
      *  .61014200,  .53608700,  .47277300,  .41849100,  .37181300,      W(Z)  477
      *  .33154400,  .29665200,  .26642700,  .24005700,  .21700400,      W(Z)  478
      *  .19676300,  .17899000,  .16328100,  .14937000,  .13701200,      W(Z)  479
      *  .12600200,  .11616400,  .10734800,  .09942700,  .09229100,      W(Z)  480
      *  .08584500,  .08000900,  .07471200,  .06989400,  .06550000,      W(Z)  481
      *  .06148000,  .05781100,  .05443900,  .05133900,  .04848500,      W(Z)  482
      *  .04585100/                                                      W(Z)  483
         DATA Z51/                                                       W(Z)  484
      *  .60715800,  .53855600,  .47899100,  .42722500,  .38216600,      W(Z)  485
      *  .34287200,  .30853000,  .27844500,  .25202400,  .22875900,      W(Z)  486
      *  .20821900,  .19003600,  .17389600,  .15953100,  .14671200,      W(Z)  487
      *  .13524200,  .12495400,  .11570200,  .10736100,  .09982400,      W(Z)  488
      *  .09295800,  .08680100,  .08116200,  .07602100,  .07132400,      W(Z)  489
      *  .06702400,  .06308000,  .05945600,  .05611800,  .05304100,      W(Z)  490
      *  .05015700/                                                      W(Z)  491
         DATA Z52/                                                       W(Z)  492
      *  .59376100,  .53200900,  .47743900,  .42927500,  .38677700,      W(Z)  493
      *  .34926000,  .31612800,  .28681500,  .26084700,  .23780000,      W(Z)  494
      *  .21736600,  .19904600,  .18274200,  .16815100,  .15506600,      W(Z)  495
      *  .14330500,  .13271100,  .12314700,  .11449500,  .10665000,      W(Z)  496
      *  .09952300,  .09303500,  .08711600,  .08170600,  .07675300,      W(Z)  497
      *  .07220800,  .06803100,  .06418600,  .06063900,  .05736300,      W(Z)  498
      *  .05433100/                                                      W(Z)  499
         DATA Z53/                                                       W(Z)  500
      *  .57239700,  .51826300,  .46948800,  .42566700,  .38641200,      W(Z)  501.
      *  .35125900,  .31951400,  .29185100,  .26675700,  .24429500,      W(Z)  502
      *  .22416800,  .20610800,  .18987800,  .17527100,  .16210000,      W(Z)  503
      *  .15020500,  .13944100,  .12968400,  .12082200,  .11276000,      W(Z)  504
      *  .10541100,  .09867600,  .09250200,  .08693600,  .08177300,      W(Z)  505
      *  .07702400,  .07268100,  .06801700,  .06489000,  .06144000,      W(Z)  506
      *  .05824300/                                                      W(Z)  507
         DATA Z54/                                                       W(Z)  508
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IV G LEVEL  21              BLK DATA            DATE = 75178          09/06/45

     *  .54545200,   .45521000,   .45655500,   .41749100,   .38190800,      W(Z)  509
     *  .34501100,   .32036800,   .29352700,   .27004000,   .24846200,      W(Z)  510
     *  .22360700,   .21134300,   .19539800,   .18095700,   .16786300,      W(Z)  511
     *  .15557500,   .14516700,   .13532600,   .12635300,   .11815600,      W(Z)  512
     *  .11066200,   .10375500,   .09749500,   .09170600,   .08637800,      W(Z)  513
     *  .08146700,   .07695300,   .07274200,   .06886300,   .06520600,      W(Z)  514
     *  .06192600/                                                          W(Z)  515
        DATA Z55/                                                           W(Z)  516
     *  .51511300,   .47653500,   .44000500,   .40562300,   .37411000,      W(Z)  517
     *  .34486800,   .31862200,   .29345300,   .27101500,   .25054900,      W(Z)  518
     *  .23185700,   .21490200,   .19941600,   .18529900,   .17242300,      W(Z)  519
     *  .16006800,   .14952700,   .14010300,   .13110600,   .12265800,      W(Z)  520
     *  .11528600,   .10835500,   .10191900,   .09601500,   .09056700,      W(Z)  521
     *  .08553200,   .08087300,   .07655700,   .07255300,   .06883400,      W(Z)  522
     *  .06537500/                                                          W(Z)  523
        DATA Z56/                                                           W(Z)  524
     *  .46322700,   .45172300,   .42107600,   .39166500,   .36382800,      W(Z)  525
     *  .33772000,   .31339700,   .29064700,   .27001600,   .25082300,      W(Z)  526
     *  .23317100,   .21695400,   .20206700,   .18640300,   .17586200,      W(Z)  527
     *  .16434900,   .15377300,   .14405400,   .13511300,   .12688300,      W(Z)  528
     *  .11925800,   .11230200,   .10584200,   .09987000,   .09434300,      W(Z)  529
     *  .08922200,   .08447200,   .08006100,   .07596000,   .07214200,      W(Z)  530
     *  .06855500/                                                          W(Z)  531
        DATA Z57/                                                           W(Z)  532
     *  .45128400,   .42616800,   .40083700,   .37591100,   .35180300,      W(Z)  533
     *  .32877700,   .30655000,   .28651700,   .26737800,   .24955600,      W(Z)  534
     *  .23300900,   .21707000,   .20349400,   .19038400,   .17827500,      W(Z)  535
     *  .16709200,   .15676500,   .14722600,   .13841200,   .13020200,      W(Z)  536
     *  .12272300,   .11574400,   .10927700,   .10328000,   .09771300,      W(Z)  537
     *  .09254100,   .08773200,   .08325400,   .07908200,   .07519100,      W(Z)  538
     *  .07155800/                                                          W(Z)  539
        DATA Z58/                                                           W(Z)  540
     *  .42038800,   .40074300,   .38016100,   .35931300,   .33807600,      W(Z)  541
     *  .31864400,   .29926100,   .28084600,   .26341800,   .24701200,      W(Z)  542
     *  .23163000,   .21725300,   .20384700,   .19136600,   .17976200,      W(Z)  543
     *  .16898000,   .15896900,   .14967400,   .14104500,   .13303300,      W(Z)  544
     *  .12559000,   .11867400,   .11224300,   .10626000,   .10068900,      W(Z)  545
     *  .09549900,   .09066600,   .08614300,   .08192500,   .07798200,      W(Z)  546
     *  .07424300/                                                          W(Z)  547
        DATA Z59/                                                           W(Z)  548
     *  .39125100,   .37621400,   .35972100,   .34247900,   .32498500,      W(Z)  549
     *  .30760900,   .29061300,   .27418000,   .25843100,   .24343900,      W(Z)  550
     *  .22924400,   .21588700,   .20327200,   .19147100,   .18042500,      W(Z)  551
     *  .17009900,   .16045700,   .15145800,   .14306300,   .13523400,      W(Z)  552
     *  .12793100,   .12111800,   .11476100,   .10882700,   .10328500,      W(Z)  553
     *  .09810700,   .09325500,   .08873500,   .08449300,   .08051900,      W(Z)  554
     *  .07679400/                                                          W(Z)  555
        DATA Z60/                                                           W(Z)  556
     *  .36443700,   .35306600,   .34000400,   .32587300,   .31116100,      W(Z)  557
     *  .29624000,   .28135200,   .26682300,   .25268100,   .23906700,      W(Z)  558
     *  .22604600,   .21365600,   .20151400,   .19082100,   .18036700,      W(Z)  559
     *  .17053400,   .16130000,   .15263700,   .14451600,   .13690800,      W(Z)  560
     *  .12978100,   .12310800,   .11685800,   .11100300,   .10551900,      W(Z)  561
     *  .10037800,   .09555800,   .09103700,   .08679400,   .08280900,      W(Z)  562
     *  .07906500/                                                          W(Z)  563
        DATA Z61/                                                           W(Z)  564
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      *  .3400260U,   .331583D0,   .3213320U,   .30983100,   .2975290D0,     W(Z) 565
      *  .2647860U,   .271681D0,   .259031D0,   .2463960D0,   .2340960D0,     W(Z) 566
      *  .22221300,   .210805D0,   .1999040D0,  .189529D0,    .1796870U,      W(Z) 567
      *  .1703710U,   .1615720C,   .1532740U,   .1454570U,    .138100DU,      W(Z) 568
      *  .131180D0,   .124674DC,   .118558D00,  .11281ODU,    .1074080U,      W(Z) 569
      *  .1023290D,   .057554D0,   .093062DU,   .088637D0,    .084859D0,      W(Z) 570
      *  .08111300/                                                           W(Z) 571
         DATA Zc2/                                                            W(Z) 572
      *  .318073D0,   .311866D0,   .303894DU,   .2945740D,    .28432700,      W(Z) 573
      *  .2734E2D0,   .262308DU,   .2510160U,   .239772DU,    .2287030D,      W(Z) 574
      *  .2179040U,   .2C744200,   .1973060DU,  .18770500,    .1784780U,      W(Z) 575
      *  .16969100,   .161343D0,   .1534290U,   .1459360D0,   .138855DU,      W(Z) 576-
      *  .1321E4D0,   .125849DU,   .11989100,   .1142720D,    .1089730D,      W(Z) 577
      *  .103677D0,   .059265DU,   .094822D0,   .090631D0,    .086677D0,      W(Z) 578
      *  .08254400/                                                           W(Z) 579
         DATA Z63/                                                            W(Z) 580
      *  .2984080U,   .295382D0,   .2877710U,   .2802320U,    .27171OD0,      W(Z) 581
      *  .26249900,   .252844D0,   .242947CU,   .2329680U,    .2230370D,      W(Z) 582
      *  .213253DU,   .2030920C,   .1944100D,   .1854460D,    .1768270D,      W(Z) 583
      *  .1685C900,   .1606080U,   .1531610U,   .146009D0,    .1392170U,      W(Z) 584
      *  .13277300,   .1266070U,   .1208650D,   .11541300,    .1102360U,      W(Z) 585
      *  .1053390U,   .1C0705DU,   .096330D0,   .09218900,    .068273D0,      W(Z) 586
      *  .08456880/                                                           W(Z) 587
         DATA Z64/                                                            W(Z) 588
      *  .2810260U,   .2777950U,   .2729680U,   .2668650U,    .2597750U,      W(Z) 589
      *  .2519530U,   .2436170U,   .2349620U,   .2261110U,    .21721900,      W(Z) 590
      *  .2083760U,   .1966060U,   .1911330U,   .1828400U,    .1748145U,      W(Z) 591
      *  .1670780U,   .1596046U,   .1525260U,   .1457210U,    .1392290D,      W(Z) 592
      *  .1330450U,   .1271610C,   .1215690U,   .1162580U,    .1112180U,      W(Z) 593
      *  .1064360U,   .1015C1DU,   .097601D0,   .09352300,    .089658DU,      W(Z) 594
      *  .08599200/                                                           W(Z) 595
         CATA Z65/                                                            W(Z) 596
      *  .2655220U,   .2632010C,   .2594350U,   .2544780U,    .2485660U,      W(Z) 597
      *  .24191400,   .2347140U,   .2271290U,   .2193020U,    .2113490U,      W(Z) 598
      *  .2033680U,   .1954380U,   .1876200U,   .1799650U,    .1725100U,      W(Z) 599
      *  .16528100,   .1582590U,   .1515760U,   .1451200U,    .1389330U,      W(Z) 600
      *  .1333610U,   .127363DC,   .1219720U,   .1168340U,    .1119420U,      W(Z) 601
      *  .1072660U,   .1028580U,   .098648DU,   .0946460U,    .09084200,      W(Z) 602
      *  .08722700/                                                           W(Z) 603
         DATA Z66/                                                            W(Z) 604
      *  .2517230U,   .2500500C,   .2470920U,   .24304200,    .2380920U,      W(Z) 605
      *  .2324200U,   .2261500C,   .2195460U,   .2126140U,    .2055040U,      W(Z) 606
      *  .1983070U,   .1510990C,   .1839400U,   .1768890U,    .1699770U,      W(Z) 607
      *  .1632370U,   .1566920U,   .1503590U,   .1442490U,    .138368DU,      W(Z) 608
      *  .1327200U,   .1273050U,   .1221210U,   .117164DU,    .112428CU,      W(Z) 609
      *  .1079090U,   .1035970U,   .0994870U,   .0955700U,    .0918380U,      W(Z) 610
      *  .08828300/                                                           W(Z) 611
         DATA Z67/                                                            W(Z) 612
      *  .2394030U,   .2381870U,   .2358380U,   .2325040U,    .2283370U,      W(Z) 613
      *  .2234820U,   .2180770U,   .2122470U,   .2061030U,    .1997440U,      W(Z) 614
      *  .1932550U,   .1607C700,   .1801630U,   .1736700U,    .1672700CU,     W(Z) 615
      *  .16009600,   .1548720U,   .1489180U,   .1431470U,    .1375609U,      W(Z) 616
      *  .1321510U,   .1270150C,   .1220420U,   .1172710U,    .112699CU,      W(Z) 617
      *  .1083220U,   .1C41360C,   .1001330U,   .0963090U,    .0926570U,      W(Z) 618
      *  .08917000/                                                           W(Z) 619
         DATA Z68/                                                            W(Z) 620
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IV G LEVEL  21              BLK DATA           DATE = 75178        09/06/45

     *  .22835500.   .22745800.   .22556900.   .22280000.   .21926800.        W(Z) 621
     *  .21509300.   .21032700.   .20525800.   .19980400.   .19411100.        W(Z) 622
     *  .18825800.   .18231100.   .17632800.   .17035700.   .16443800.        W(Z) 623
    _*  .15886040.   .15286260.   .14729200.   .14185100.   .13657100.        W(Z) 624
     *  .13145500.   .12652200.   .12176200.   .11718000.   .11277500.        W(Z) 625
     *  .10854600.   .10446900.   .10060100.   .09687600.   .09331000.        W(Z) 626
     *  .08985800/                                                            W(Z) 627
       DATA Z69/                                                              W(Z) 628
     *  .21835900.   .21772200.   .21618100.   .21385800.   .21084300.        W(Z) 629
     *  .20723200.   .20311900.   .19859400.   .19374100.   .18863800.        W(Z) 630
    -*-.18335400.   .17792000.   .17248000.   .16699000.   .16151900.         W(Z) 631
     *  .15609900.   .15075800.   .14551800.   .14039500.   .13540300.        W(Z) 632
     *  .13055300.   .12585100.   .12130300.   .11691100.   .11267600.        W(Z) 633
     *  .10859700.   .10467400.   .10090500.   .09726400.   .09381000.        W(Z) 634
     *  .09047900/                                                            W(Z) 635
       DATA Z70/                                                              W(Z) 636
     *  .20937700.   .20885400.   .20757700.   .20560700.   .20301400.        W(Z) 637
     *  .19987300.   .19626200.   .19225600.   .18792700.   .18334400.        W(Z) 638
     *  .17854800.   .17365400.   .16865100.   .16360300.   .15854700.        W(Z) 639
     *  .15351500.   .14853400.   .14362500.   .13880700.   .13409400.        W(Z) 640
     *  .12949800.   .12502700.   .12068800.   .11648400.   .11241900.        W(Z) 641
     *  .10845300.   .10470700.   .10105800.   .09754600.   .09416800.        W(Z) 642
     *  .09009210/                                                            W(Z) 643
       DATA Z71/                                                              W(Z) 644
     *  .20115700.   .20074200.   .19966900.   .19798000.   .19573200.        W(Z) 645
     *  .19258400.   .18975800.   .18623900.   .18236800.   .17824300.        W(Z) 646
     *  .17391800.   .16944500.   .16486600.   .16022300.   .15555100.        W(Z) 647
     *  .15088000.   .14623600.   .14164000.   .13711300.   .13266700.        W(Z) 648
     *  .12831700.   .12407100.   .11993600.   .11591900.   .11202300.        W(Z) 649
     *  .10824900.   .10460600.   .10107600.   .09767400.   .09439500.        W(Z) 650
     *  .09012360/                                                            W(Z) 651
       DATA Z72/                                                              W(Z) 652
     *  .19363000.   .19329200.   .19237600.   .19091500.   .18895100.        W(Z) 653
     *  .18653200.   .18371600.   .18053400.   .17706100.   .17334000.        W(Z) 654
     *  .16941800.   .16533500.   .16114500.   .15687200.   .15255300.        W(Z) 655
     *  .14821700.   .14388800.   .13958800.   .13533500.   .13114600.        W(Z) 656
     *  .12703100.   .12300300.   .11906800.   .11523300.   .11150300.        W(Z) 657
     *  .10788100.   .10437000.   .10066900.   .09768000.   .09450200.        W(Z) 658
     *  .09143400/                                                            W(Z) 659
       DATA Z73/                                                              W(Z) 660
     *  .18070400.   .18042100.   .18563000.   .18435400.   .18262600.        W(Z) 661
     *  .18048400.   .17797000.   .17512800.   .17200300.   .16863700.        W(Z) 662
     *  .16507200.   .16134500.   .15750200.   .15356700.   .14957200.        W(Z) 663
     *  .14554500.   .14151000.   .13748800.   .13349500.   .12954800.        W(Z) 664
     *  .12566000.   .12184000.   .11809900.   .11444200.   .11087500.        W(Z) 665
     *  .10740300.   .10402700.   .10075100.   .09757500.   .09449900.        W(Z) 666
     *  .09152300/                                                            W(Z) 667
       DATA Z74/                                                              W(Z) 668
     *  .18030200.   .18006100.   .17936900.   .17824500.   .17671500.        W(Z) 669
     *  .17480800.   .17255000.   .17000600.   .16718400.   .16413200.        W(Z) 670
     *  .16086600.   .15746000.   .15394800.   .15032000.   .14662300.        W(Z) 671
     *  .14268200.   .13912000.   .13535700.   .13160900.   .12789200.        W(Z) 672
     *  .12421900.   .12060000.   .11704500.   .11356000.   .11015300.        W(Z) 673
     *  .10682700.   .10358600.   .10043300.   .09736900.   .09439600.        W(Z) 674
     *  .09151300/                                                            W(Z) 675
       DATA Z75/                                                              W(Z) 676
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IV G LEVEL  21              BLK DATA            DATE = 75178            09/06/45

    *  .17436200,  .17416200,  .17354200,  .17254500,  .17118100,        W(Z)  677
    *  .16947500,  .16745500,  .16515100,  .16269600,  .15982100,        W(Z)  678
    *  .15685800,  .15373800,  .15049000,  .14714100,  .14371700,        W(Z)  679
    *  .14023900,  .13673100,  .13320900,  .12969100,  .12619200,        W(Z)  680
    *  .12272300,  .11925600,  .11591900,  .11260200,  .10934900,        W(Z)  681
    *  .10616600,  .10305700,  .10002600,  .09707300,  .09420200,        W(Z)  682
    *  .09141300/                                                        W(Z)  683
       DATA Z76/                                                         W(Z)  684
    *  .16883000,  .16864500,  .16810200,  .16721200,  .16599000,        W(Z)  685
    *  .16445600,  .16263300,  .16054800,  .15822700,  .15569800,        W(Z)  686
    *  .15258800,  .15012400,  .14713200,  .14403800,  .14086200,        W(Z)  687
    *  .13762800,  .13435400,  .13105800,  .12775500,  .12446000,        W(Z)  688
    *  .12118500,  .11794000,  .11473500,  .11157800,  .10847400,        W(Z)  689
    *  .10543100,  .10245100,  .09953800,  .09669500,  .09392700,        W(Z)  690
    *  .09123000/                                                        W(Z)  691
       DATA Z77/                                                         W(Z)  692
    *  .16366200,  .16345800,  .16301100,  .16221100,  .16111100,        W(Z)  693
    *  .15972500,  .15807500,  .15618100,  .15406600,  .15175800,        W(Z)  694
    *  .14927100,  .14663700,  .14387800,  .14101400,  .13806700,        W(Z)  695
    *  .13505600,  .13199900,  .12891300,  .12581200,  .12270900,        W(Z)  696
    *  .11961700,  .11654500,  .11350300,  .11050000,  .10754000,        W(Z)  697
    *  .10463100,  .10177700,  .09898100,  .09624700,  .09357700,        W(Z)  698
    *  .09095730/                                                        W(Z)  699
       DATA Z78/                                                         W(Z)  700
    *  .15882100,  .15867300,  .15823500,  .15751300,  .15651600,        W(Z)  701
    *  .15526000,  .15376000,  .15203400,  .15010200,  .14798500,        W(Z)  702
    *  .14570300,  .14327700,  .14072700,  .13807400,  .13533600,        W(Z)  703
    *  .13253000,  .12967400,  .12678200,  .12386900,  .12094700,        W(Z)  704
    *  .11802700,  .11512000,  .11223400,  .10937700,  .10655600,        W(Z)  705
    *  .10377700,  .10104400,  .09836200,  .09573400,  .09316200,        W(Z)  706
    *  .09064900/                                                        W(Z)  707
       DATA Z79/                                                         W(Z)  708
    *  .15427300,  .15414000,  .15374300,  .15308600,  .15218300,        W(Z)  709
    *  .15104000,  .14967200,  .14809400,  .14632400,  .14438000,        W(Z)  710
    *  .14227500,  .14003500,  .13768000,  .13521800,  .13267100,        W(Z)  711
    *  .13008400,  .12738400,  .12467300,  .12193500,  .11918200,        W(Z)  712
    *  .11642500,  .11367300,  .11093500,  .10821800,  .10553000,        W(Z)  713
    *  .10287600,  .10026900,  .09768800,  .09516300,  .09268800,        W(Z)  714
    *  .09026500/                                                        W(Z)  715
       DATA Z80/                                                         W(Z)  716
    *  .14996200,  .14987100,  .14951000,  .14891300,  .14808600,        W(Z)  717
    *  .14704400,  .14575200,  .14434600,  .14272100,  .14093100,        W(Z)  718
    *  .13899300,  .13692200,  .13473500,  .13244800,  .13007600,        W(Z)  719
    *  .12763300,  .12513300,  .12259100,  .12001600,  .11742200,        W(Z)  720
    *  .11481700,  .11221200,  .10961400,  .10703100,  .10446900,        W(Z)  721
    *  .10193500,  .09943300,  .09696800,  .09454300,  .09216200,        W(Z)  722
    *  .08982600/                                                        W(Z)  723
       END                                                              W(Z)  724
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```
        DIMENSION HEADS(20)
        DIMENSION HTSTOR(30),ENSTOR(30),IAUSTR(30)
        DIMENSION ANG(2500),HT(2500),PLOTX(2500),PLOTY(2500),
       *XPLT(4),YPLT(4),BUFF(1000)
        NCASE=0
        ISTART=1
        STMAX=-1000.
        WRITE(6,81527)
 81527 FORMAT(1H1///)
        CALL PLOTS(BUFF,4000,10)
        CALL PLOT(0.,-12.,3)
        CALL PLOT(0.,-11.5  ,23)
C
C       READ IN CONTROL PARAMETERS
C
 88366 READ(20,END=4954)SLIT,PLTMIN,PLTMAX,DELPLT,DLAM,YHGT,NLINES,END,
       *TL,TA,EL,IPLOT1,IPLOT2
       *,LIR2,APRIME
       *,TAU
       *,HEADS
        TRAF=(-1)**LIR2
C       -
C       READ IN WAVENUMBER, TRANSMISSION PAIRS, CONVERT WAVENUMBERS
C       TO WAVELENGTH AND DETERMINE MAXIMUM TRANSMISSION
C
        DO 837 ICARD=1,NLINES
        READ(20)ANG(ICARD),HT(ICARD)
        IF(HT(ICARD).LT.0.)HT(ICARD)=0.
        STMAX=AMAX1(STMAX,HT(ICARD))
        ANG(ICARD)=(1.E+08)/ANG(ICARD)
    837 CONTINUE
        NCASE=NCASE+1
        II=NLINES
        PLTMIN=ANG(1)
        PLTMAX=ANG(II)
        WIDE=2.*DLAM
        PLTMIN=PLTMIN-2.*WIDE
        PLTMAX=PLTMAX+2.*WIDE
        DELTA=STMAX/5.
     35 CONTINUE
C
C       PRODUCE THE ZERO SLIT WIDTH PLOTS WHEN IPLOT1=1
C
        IF(IPLOT1.EQ.0)GO TO 66001
        TEST=(PLTMAX-PLTMIN)/DELPLT
        ILG=TEST
        ILG=ILG+2
        HLG=ILG
        XPLT(3)=PLTMIN
        XPLT(4)=DELPLT
        YPLT(3)=0.
        YPLT(4)=DELTA
        BOOZE=YPLT(4)+10.
        CALL AXIS(0.,0.,'A ',-1,HLG,0.,XPLT(3),XPLT(4),10.)
        YPLT(1)=0.
        DO 50 I=1,II
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        RLAM=ANG(I)
        IF(PLTMIN.GT.RLAM.OR.PLTMAX.LT.RLAM)GO TO 50
        YPLT(2)=AMIN1(HT(I),BCOZE)
        XPLT(1)=RLAM
        XPLT(2)=XPLT(1)
        CALL LINE(XPLT,YPLT,2,1,0,1)
    50  CONTINUE
        CALL PLOT(RLG+2.,0.,-3)
  6001 CONTINUE
C
C       PRODUCE THE ACTUAL SPECTRA PLOT
C
        ISAVE=1
        KKOUNT=1
        DELLAM=(PLTMAX-PLTMIN)/2499
        PP1=PLTMIN-DELLAM
   991  LOOK=ISAVE-1
        IF(LOOK.LE.0)LOOK=1
C
C       CHOOSE A POINT ALONG THE PLOT AXIS AND SET AN INTERVAL OF WIDTH
C       EQUAL TO THE SLIT WIDTH ON EITHER SIDE
C
        P1=PP1+KKOUNT*DELLAM
        P2=P1+WIDE
        XLAM=(P1+P2)*.5
        KOUNT=1
C
C       THIS LOOP DETERMINES WHICH LINES LIE IN THE CHOSEN INTERVAL
C
        DO 9969 I=LOOK,II
        IF(ANG(I).GT.P2)GO TO 992
        IF(ANG(I).LT.P1)GO TO 9969
        IF(KOUNT.EQ.1)ISAVE=I
        KOUNT=KOUNT+1
  9969  CONTINUE
   992  NUPTS=KOUNT-1
C
C       THE FOLLOWING STATEMENTS SIMULATE THE TRIANGULAR SLIT FUNCTION
C       BY SUMMING THE CONTRIBUTIONS OF ALL THE LINES IN THE INTERVAL
C
        IF(NUPTS.EQ.0)GO TO 9974
        SUMMER=0.
        IPN1=ISAVE+NUPTS-1
        DO 9934J JEL=ISAVE,IPN1
        TRIAUD=HT(JEL)*(DLAM-ABS(XLAM-ANG(JJL)))/DLAM
  9934J SUMMER=SUMMER+AMAX1(0.,TRIAUD)
        PLOTX(KKOUNT)=XLAM
        PLOTY(KKOUNT)=SUMMER
        KKOUNT=KKOUNT+1
        IF(KKOUNT.EQ.2501)GO TO 77
        GO TO 991
  9974  PLOTX(KKOUNT)=XLAM
        PLOTY(KKOUNT)=0.
        KKOUNT=KKOUNT+1
        IF(ANG(II).LT.P1)GO TO 77
        IF(KKOUNT.EQ.2501)GO TO 77
```

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              GU TO 991
           77 II=KKOUNT-I
              N=II
              TTRAF=.5*TRAF*DLAM
              DO 88 I=1,N
           88 PLOTX(I)=PLOTX(I)+TTRAF
              TEST=(PLTMAX-PLTMIN)/DELPLT
              ILG=TEST
              ILG=ILG+2
              RLG=ILG
      C
      C
      C      DETERMINE THE MAXIMUM VALUE CF THE SPECTRAL CURVE AND IF THIS
      C      IS THE FIRST CURVE COMPUTED. THE Y AXIS SCALE FACTOR IS CALCULATED
      C
              SPMAX=-100.
              DO 800 I=1,N
              IF(PLOTY(I).LT.SPMAX)GO TO 800
              SPMAX=PLOTY(I)
          800 CONTINUE
              IF(ISTART.EQ.1)DELYP=SPMAX/YHGT
          801 PLOTY(N+1)=0.
              PLOTY(N+2)=DELYP
              PLOTX(N+1)=PLTMIN
              PLOTX(N+2)=DELPLT
              VALMAX=10.*PLOTY(N+2)
              DO 65395 MONDAY=1,N
              IF(PLOTY(MONDAY).GT.VALMAX)PLOTY(MONDAY)=VALMAX
        65395 CONTINUE
              NP2=N+2
              WRITE(40)NP2,(PLOTX(L),PLOTY(L),L=1,NP2)
      C
      C      PRODUCE A SEPARATE PLOT FOR EACH VALUE OF ENO IF IPLOT2=1
      C
              IF(IPLOT2.EQ.0)GO TO 66002
              CALL AXIS(0.,0.,'A',-1,RLG,0.,PLOTX(N+1),PLOTX(N+2),10.)
              CALL SYMBOL(.5,5.0,.1,'NO=',0.,3)
              CALL PLTFLT(-0.,-0.,-0.,ENO,6.,3)
              CALL LINE(PLOTX,PLOTY,N,1,0,1)
              CALL PLOT(RLG+2.,0.0,-3)
        66002 CONTINUE
              ISTART=0
              TAUSTR(NCASE)=TAU
              HISTOR(NCASE)=SPMAX/DELYP
              ENSTOR(NCASE)=ENO
              GO TO 88388
         4994 CONTINUE
      C
      C      PRODUCE THE FINAL SPECTRA PLOT
      C
              CALL AXIS(0.,0.,'WAVELENGTH',-10,RLG,0.,PLTMIN,DELPLT,10.)
              CALL SYMBOL(.5,5.9,.1,HEADS,0.,80)
              CALL SYMBOL(.5,5.5,.1,'TE=',0.,3)
              CALL NUMBER(-0.,-0.,-0.,TE,0.,-1)
              CALL SYMBOL(.5,5.3,.1,'TA=',0.,3)
              CALL NUMBER(-0.,-0.,-0.,TA,0.,-1)
              CALL SYMBOL(.5,5.1,.1,'L= ',0.,3)
```

```
      CALL NUMBER(-0.,-0.,-0.,EL,0.,1)
      CALL SYMBOL(.5,6.9,.1,3HA'=,0.,3)
      CALL NUMBER(-0.,-0.,-0.,APRIME,0.,5)
      CALL SYMBOL(-.285715,6.7,.1,'  NO  MAX HT  TAU',0.,19)
      CALL SYMBOL(-.285715,8.55,.1,'          (IN)',0.,13)
      DO 78 I=1,NCASE
      YB=8.6-.15*I
      CALL PLTFLT(-.385715,YB,.1,ENSTOR(I),0.,2)
      CALL NUMBER(.42914,YB,.1,HTSTCR(I),0.,2)
      CALL NUMBER(1.028578,YB,.1,TALSTR(I),0.,3)
   78 CONTINUE
      ENDFILE 40
      REWIND 40
  150 READ(40,END=4995)NP2,(PLOTX(L),PLOTY(L),L=1,NP2)
      N=NP2-2
      CALL LINE(PLOTX,PLOTY,N,1,0,1)
      GO TO 150
 4995 CALL PLOT(RLG+2.,0.,-3)
 4997 CALL PLOT(0.0,999)
      STOP
      END
```

NOMENCLATURE

$\bar{T}_j$	Transmission of spectral line (designated j) through a medium, intensity units
ν_i, ν_j	Wavenumber of the ith or jth spectral line, cm^{-1}
I_{ν_j}	Intensity of source spectral line at wavenumber, ν_j, intensity units
k_{ν_j}, k_{ν_i}	Absorption coefficient for the spectral line at wavenumber, ν_j or ν_i, cm^{-1}
ℓ	Absorption path length, cm
ν	Wavenumber, cm^{-1}
$I^\circ_{\nu_j^\circ}$	Intensity of source spectral line at center wavenumber, ν_j°, intensity units
ν_i°, ν_j°	Center wavenumber of the ith or jth spectral line, cm^{-1}
$(\Delta_s \nu_i)_D$, $(\Delta_s \nu_j)_D$	Doppler width at half maximum intensity of the ith or jth source spectral line, cm^{-1}
κ	Boltzmann's constant, $0.6952\ cm^{-1}\ K^{-1}$
T_s	Temperature of gas in light source, K
M_s, M_a	Mass of molecules in light source and absorber, respectively, gm
c	Velocity of light, 3×10^{10} cm/sec
$k_{\nu_j^\circ}$, $k_{\nu_i^\circ}$	Absorption coefficient at center wavenumber, ν_j° or ν_i°, cm^{-1}
a′	Spectral line broadening parameter (ratio of collisional to Doppler line widths)
y	Dummy variable of integration
ω	Doppler frequency function, $\dfrac{2(\nu_j - \nu_j^\circ)}{(\Delta_a \nu_j)_D}\sqrt{\ell n\ 2}$
$(\Delta_a \nu_j)_D$, $(\Delta_a \nu_i)_D$	Doppler width at half maximum absorption coefficient, $k_{\nu_j^\circ}$, of the ith or jth absorption line, cm^{-1}

$(\Delta_a \nu_j)_L$	Lorentz width at half maximum intensity of the jth absorbing spectral line, cm^{-1}
Z_L	Effective collision frequency for spectral line broadening, sec^{-1}
T_a	Temperature of absorber gas, °K
$\overline{T}_{\Delta\nu}$	Transmission over the frequency interval $\Delta\nu$ through a medium, intensity units
$t_{\Delta\nu}$	Transmissivity over the frequency interval $\Delta\nu$; ratio of incident to transmitted intensity
$\Delta\nu$	Wavenumber increment, cm^{-1}
e	Electronic charge, 4.80×10^{-10} esu
m	Electron mass, 9.11×10^{-28} gm
$N_{J''}$	Number density of molecules in the lower state, J'', cm^{-3}
$f_{J'J''}$	Oscillator strength for the transition from the upper state J' to the lower state J''
h	Planck's constant, 6.625×10^{-27} erg sec
B_{v_0}	Rotational constant for the vth vibrational state (ground state, $v = 0$), cm^{-1}
J''	Rotational quantum number for the lower state
$F(J'')$	Rotational energy of the J''th rotational state, cm^{-1}
N_0	Total number density of molecules, cm^{-3}
$f_{v'v''}$	Band oscillator strength for the $v' \leftrightarrow v''$ transition
$\nu_{J'J''}$	Wavenumber of the line corresponding to the transition $v'J' \to v''J''$, cm^{-1}
$\nu_{v'v''}$	Wavenumber at the bandhead of the (v', v'') band, cm^{-1}
$\delta_{J''J'}$	Rotational strength, or Hönl-London factor, for the $v'J' - v''J''$ vibrational - rotational transition
S	Total electron spin quantum number
N_ℓ	Number density of molecules ℓ other than the absorbing molecule in the absorbing medium, cm^{-3}

σ_{ℓ}^{2}	Effective collisional cross section for the broadening process by the ℓth type molecule, cm^2
N/ℓ	Mass of the ℓth type molecule, gm
λ_{j}^{o}	Wavelength at line center of the jth spectral line, cm
p_{ℓ}	Partial pressure of the ℓth type molecule, torr
M_{f}	Mass of the fth type molecule, gm
C_{j}	Line broadening constant for the jth spectral line, K/torr or K/atm
C	Average line broadening constant for all spectral lines in a given band, K/atm